

DYNAMICS OF A SIMPLE QUANTUM SYSTEM IN A COMPLEX ENVIRONMENT

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Abstract

We present a theory for the dynamical evolution of a quantum system coupled to a complex many-body intrinsic system/environment. By modelling the intrinsic many-body system with parametric random matrices, we study the types of effective stochastic models which emerge from random matrix theory. Using the Feynman–Vernon path integral formalism, we derive the influence functional and obtain either analytical or numerical solutions for the time evolution of the entire quantum system. We discuss thoroughly the structure of the solutions for some representative cases and make connections to well known limiting results, particularly to Brownian motion, Kramers classical limit and the Caldeira–Leggett approach.

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I. INTRODUCTION

Quantum dissipation is a problem with such a long history and such a multitude of results that even a cursory review will not make justice to the numerous contributions of a large number of authors over several decades. We recommend the reader to consult Refs. [1–9,11] and the references therein. In spite of this impressive effort, many people do not consider the problem of quantum dissipation a solved issue, and its character and microscopic origin still call for the attention of a large community across many, if not all, subfields of physics. The present paper represents a continuation of our effort to understand the character of energy flow between the slow degrees of freedom and the intrinsic degrees of freedom in many-body systems. Our initial motivation was to understand the “irreversible” time evolution of the large amplitude nuclear collective motion [6–10] and for that reason we have adopted a traditionally nuclear physics approach. The large body of evidence, both experimental and theoretical, suggests that many Fermion systems can be described reasonably well within the framework of a random matrix formalism. Another way of saying the same thing is that a many Fermion system is predominantly a quantum chaotic system and thus a random matrix approach is a natural approach. At the same time, both theory and experiment strongly suggest that there are some degrees of freedom, which are not chaotic and usually are referred to as collective or shape. However these collective degrees of freedom are coupled with a large number of non-collective degrees of freedom and as a result a rather generic situation results: a relatively small quantum system in contact with an “environment”. Even though the whole system is finite and in a strict sense there is no irreversible behaviour in this case, for all practical purposes the time evolution of the collective or slow quantum system has the character of quantum dissipative dynamics. In our formulation, we will neglect other physical mechanisms which lead to dissipative contributions, such as particle evaporation or coupling to electromagnetic fields. This can be viewed as limiting the present study to shorter time scales. Such phenomena can in principle be introduced into the formalism, but we shall not attempt it here. We shall not either try here to defend the legitimacy of such a terminology (dissipation), the issue at stake however is unquestionably sound. The reader will recognize easily that the problem we address here is typical and under different guises appears in many subfields of physics.

As an introduction, let us consider for the moment that a certain simple system interacts with some relatively large (but finite) many-body system. The question is: can one describe the dynamical behaviour of the simple system using for example an equation of the form

$$M \frac{d^2 X}{dt^2} = - \frac{dU(X)}{dX} - M\gamma \frac{dX}{dt} + f(X, t) \quad (1.1)$$

as in the case of a Brownian particle, if in the absence of the interaction the Hamiltonian of the system is

$$H_0(X, P) = \frac{P^2}{2M} + U(X) \quad (1.2)$$

and where γ is a friction coefficient and $f(X, t)$ is a Langevin-like force? The force $f(X, t)$ can in principle depend not only on time but on position as well, and in this way one can

describe a large variety of physical situations, ranging from diffusion to localization [11]. If one were to start from a description of the entire system (reservoir plus simple system) with a Hamiltonian

$$H(X, P, x, p) = H_0(X, P) + H_1(X, x, p), \quad (1.3)$$

where $H_1(X, x, p)$ describes the reservoir and its interaction with our system, under what circumstances could one derive an equation of motion like Eq.(1.1)? Moreover, does the fluctuating force have Gaussian character or not? Since our approach is a fully quantum mechanical one, we shall be able to answer another important question, on the specific role played by the quantum effects. As we shall show, the classical results are recovered when the appropriate limits are taken, however, the classical limit is not at all a trivial one nor is it reached in a simple fashion. If one were to take the approach of postulating that an equation of the type Eq. (1.1) governs the dynamics and assume for example that the fluctuation properties of $f(X, t)$ are Gaussian in character, then the entire powerful apparatus developed for Brownian motion could be then invoked [11]. But such an approach would leave unanswered the main questions of whether one can describe in this way collective degrees of freedom in a finite closed system, like atomic nuclei.

We address this problem using a well known approach based on the double path integral formulation of Feynman and Vernon [1]. Our original input is in the functional form of the influence functional, which arises from a parametric random matrix description of the “environment”. This has been attempted earlier in Ref. [5]. The functional form for the influence functional we determine is qualitatively different from the popular Caldeira–Leggett type derived by Feynman and Vernon [1]. The parameters which define the influence functional have a rather simple and intuitive meaning from a microscopic point of view and we refer the reader to earlier publications for details and discussions [5–10]. It comes as no surprise than that under such circumstances the dynamical evolution of a quantum dissipative system in our case has new features as well, as we shall amply exemplify in the body of the paper. Here we restrict our attention to the Markovian limit only and we hope to address the important problem of memory effects in the future. In spite of its physical restrictions (high temperature limit for the intrinsic system) this limit shows already the qualitative differences with the previously known approaches.

The paper is organized as follows. In Section II we discuss the time evolution equation for the density matrix of the “slow” quantum system coupled to a complex many–body system. In Section III we show that, at high temperatures, the evolution equation for the density matrix can be brought to the Kramers form, when the classical limit is taken. Sections IV–VII discuss exact solutions to the evolution equations for certain potentials. Section VIII is devoted to the study of the tunneling problem. A short summary and discussion of the results is given in the final Section.

II. EVOLUTION EQUATION FOR THE DENSITY MATRIX

In this section we discuss the description of the internal degrees of freedom (or complex environment) through parametric random matrix theory, and derive the equation of motion for the density matrix of the slow degrees of freedom by integrating over the internal states.

A. Random Matrix Model

The basic assumption concerning the intrinsic states is that there are no governing constants of the motion, so that the dynamics is chaotic. This has been seen to be the general situation in studies of many-body systems, from nuclei to molecules, so it is reasonable to approach the modelling of these degrees of freedom with random matrices, suitably tailored to the problem. The generic form of the Hamiltonian governing the dynamics of a “slow” quantum system coupled to a complex environment is described as follows

$$H(X, x) = H_0(X) + H_1(X, x) = \frac{P_X^2}{2M} + U(X) + H_1(X, x). \quad (2.1)$$

We shall often refer to X as “shape” variables, since in large amplitude collective nuclear motion it represents the collective coordinates which characterize the nuclear mean field.

The part of the total Hamiltonian Eq. (2.1) which depends on the intrinsic coordinates $H_1(X, x)$ is defined as a matrix, whose matrix elements depend parametrically on the “slow” coordinate X

$$[H_1(X)]_{ij} = [h_0]_{ij} + [h_1(X)]_{ij}. \quad (2.2)$$

h_0 is taken to be diagonal and defines the average density of states, with $\langle k|h_0|l \rangle = [h_0]_{kl} = \varepsilon_k \delta_{kl}$. We refer in the main text to these eigenstates as “typical states” of the intrinsic system with an energy ε . One can think of h_0 as a Hamiltonian describing a “bath” or a “reservoir” and of $h_1(X)$ as a Hamiltonian describing the interaction between the “bath/reservoir” and the “slow” system. Whereas in statistical physics the interaction between the thermostat and the system under consideration is assumed to be negligible, we shall not make such an approximation here. As a matter of fact, for the physically interesting situations we envision, this coupling term can be large. This fact alone leads to significant differences of various distributions when compared with the corresponding results of traditional approaches.

For an intrinsic subsystem with a large number of degrees of freedom, the average density of states,

$$\rho(\varepsilon) = \overline{\text{Tr} \delta(H_1(X) - \varepsilon)}, \quad (2.3)$$

for each given shape X increases sharply with energy. The overline denotes here a procedure for extracting the smooth part of $\rho(\varepsilon)$ as a function of energy, which amounts essentially to an ensemble average, to be introduced below. For a many Fermion system, $\rho(\varepsilon)$ has a roughly exponential behaviour. Recall that $\ln \rho(\varepsilon)$ is approximately proportional to the thermodynamic entropy of the intrinsic system, which is an extensive quantity. The fact that the average density of states for the intrinsic subsystem has such a behavior is a key element of the entire approach. This is equivalent to stating that the intrinsic subsystem has a large heat capacity and thus can play the role of a “reservoir”, although not necessarily ideal. In principle $\rho(\varepsilon)$ can be X -dependent as well, but we shall ignore this aspect here. Without an X -dependence of the average density of states, mechanical work cannot be performed on or by the model environment we study here, and only heat exchange is allowed.

In Refs. [6–10] we discussed the reasons why one chooses this specific form of the Hamiltonian. In the basis of the eigenstates of h_0 , we define $h_1(X)$ as a parameter dependent, $N \times N$ real Gaussian random matrix, which is completely specified by its first two moments

$$\begin{aligned}\overline{[h_1(X)]_{kl}} &= 0, \\ \overline{[h_1(X)]_{ij}[h_1(Y)]_{kl}} &= [\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}]\mathcal{G}_{ij}(X - Y).\end{aligned}\tag{2.4}$$

The overline stands for statistical averages over the ensemble of random Gaussian matrices from the Gaussian Orthogonal Ensemble (GOE) [12]. $\mathcal{G}_{ij}(X - Y)$ can be taken as a “bell shaped” correlation function with a characteristic width X_0 , or, in some physically interesting cases even periodic, with period $\propto X_0$. The fact that this correlator is “translational invariant” is not a crucial limitation, and a general form can be adopted without any significant changes in the formalism. We limit our analysis to the GOE case only for the sake of simplicity of the argument, as any other Gaussian ensemble can be treated in a similar manner. The dependence on i, j allows for the description of banded matrices, where an effective number of states $N_0 \leq N$ are coupled by $h_1(X)$. It is convenient to use an explicit parameterization, which incorporates the average density of states and the bandwidth of the statistical fluctuations explicitly [5]:

$$\mathcal{G}_{ij}(X) = \frac{\Gamma^\downarrow}{2\pi\sqrt{\rho(\varepsilon_i)\rho(\varepsilon_j)}} \exp\left[-\frac{(\varepsilon_i - \varepsilon_j)^2}{2\kappa_0^2}\right] G\left(\frac{X}{X_0}\right).\tag{2.5}$$

Here $G(x) = G(-x) = G^*(x) \leq 1$, $G(0) = 1$, and the spreading width Γ^\downarrow , κ_0 (linked with the effective band width $N_0 \approx \kappa_0\rho(\varepsilon)$) and X_0 are characteristic of the intrinsic system. Even though it is not necessary, in this paper we shall consider a particular form for $G(x)$, namely $G(x) = \exp(-x^2/2)$.

To complete the tailoring of the random matrices, we require a realistic average density of states for the reservoir. It is reasonable to assume that in a suitable energy interval, ρ has the behaviour [5]

$$\rho(\varepsilon) = \rho_0 \exp(\beta\varepsilon), \quad \beta = \frac{1}{T} = \frac{d}{d\varepsilon} \ln \rho(\varepsilon).\tag{2.6}$$

β can thus be interpreted as the thermodynamic temperature of the intrinsic system. As β is independent of the internal excitation energy ε , this particular type of intrinsic quantum system plays the role of a “perfect” thermal quantum reservoir. We note in passing that even though the temperature of the “reservoir” remains constant throughout the entire dynamical evolution of the whole system, one should not conclude from this that the “reservoir” is in thermal equilibrium. As we have shown explicitly in Refs. [8,9] the population of various energy levels of a uniformly driven “reservoir” is far from an equilibrium Boltzmann distribution. The parameters of the present construction are summarized in Table I.

B. Influence Functional

The quantum description of our coupled system will be treated through the path integral construction of the density matrix. According to Feynman and Vernon [1], one can write the following double path integral representation for the density matrix of the entire system

$$\begin{aligned}
\mathcal{R}(X, x, Y, y, t) &= \int dX_0 dY_0 \psi(X_0) \psi^*(Y_0) \int_{X(0)=X_0}^{X(t)=X} \mathcal{D}X(t) \int_{Y(0)=Y_0}^{Y(t)=Y} \mathcal{D}Y(t) \\
&\times \exp \left\{ \frac{i}{\hbar} [S_0(X(t)) - S_0(Y(t))] \right\} \\
&\times \langle x | T \exp \left[-\frac{i}{\hbar} \int_0^t dt' H_1(X(t')) \right] | \phi \rangle \langle \phi | T_a \exp \left[\frac{i}{\hbar} \int_0^t dt'' H_1(Y(t'')) \right] | y \rangle, \quad (2.7)
\end{aligned}$$

where T and T_a represent the time ordering and time anti-ordering operators respectively. In this representation, we have used a particular form for the initial state wave function,

$$\Psi(X, x) = \psi(X) \phi(x). \quad (2.8)$$

Other choices are equally possible, such as an initial density matrix. By introducing the influence functional $\mathcal{L}(X(t), Y(t), t)$

$$\mathcal{L}(X(t), Y(t), t) = \langle \phi | \left\{ T_a \exp \left[\frac{i}{\hbar} \int_0^t dt'' H_1(Y(t'')) \right] \right\} \left\{ T \exp \left[-\frac{i}{\hbar} \int_0^t dt' H_1(X(t')) \right] \right\} | \phi \rangle \quad (2.9)$$

one readily obtains the following double path integral representation for the density matrix for the “slow” subsystem

$$\begin{aligned}
\rho(X, Y, t) &= \int dX_0 dY_0 \psi(X_0) \psi^*(Y_0) \int_{X(0)=X_0}^{X(t)=X} \mathcal{D}X(t) \int_{Y(0)=Y_0}^{Y(t)=Y} \mathcal{D}Y(t) \\
&\times \exp \left\{ \frac{i}{\hbar} [S_0(X(t)) - S_0(Y(t))] \right\} \mathcal{L}(X(t), Y(t), t). \quad (2.10)
\end{aligned}$$

The formulation of the problem through a path integral representation serves only as a very convenient vehicle to obtain an evolution equation for the density matrix $\rho(X, Y, t)$.

C. Evolution Equations

The evolution equation for the influence functional $\mathcal{L}(X(t), Y(t), t)$ has been solved in Ref. [8–10] for the case $N \rightarrow \infty$ and the case when the “temperature” of the reservoir is infinite. In Appendices A–D we compute the first order correction in β to the influence functional in the adiabatic limit, when the characteristic time scale of the “reservoir” \hbar/κ_0 is significantly shorter than the characteristic time scale of the slow system for which we derive the dynamical evolution equation. We thus obtain for the influence functional

$$\begin{aligned}
\mathcal{L}(X(t), Y(t)) &= \exp \left\{ \frac{\Gamma^\downarrow}{\hbar} \int_0^t ds \left[G \left(\frac{X(s) - Y(s)}{X_0} \right) - 1 \right] \right\} \\
&\times \exp \left\{ \frac{i\beta\Gamma^\downarrow}{4X_0} \int_0^t ds [\dot{X}(s) + \dot{Y}(s)] G' \left(\frac{X(s) - Y(s)}{X_0} \right) \right\}. \quad (2.11)
\end{aligned}$$

where $G'(x) = dG(x)/dx$. The physical significance of all other quantities entering this expression has been explained and discussed at length in Refs. [6–9], and is briefly summarized in Table I. It is worth noting that the functional form of the influence functional derived by us is different from the Caldeira–Leggett form [2], which is a quadratic expression in $X(t)$ and

$Y(t)$. If we were to use only the first term in a Taylor expansion of $G[(X(s) - Y(s))/X_0] - 1$, we would obtain an expression similar to Caldeira–Leggett form for the influence functional. However, the present form of the influence functional leads in the classical limit to a velocity dependent frictional force, see Ref. [8,9].

By combining the double path integral representation for the density matrix $\rho(X, Y, t)$ with the above expression for the influence functional in the adiabatic approximation one readily obtains that the density matrix satisfies the following Schrödinger like equation (for similar examples see Refs. [2,4])

$$i\hbar\partial_t\rho(X, Y, t) = \left\{ \frac{P_X^2}{2M} - \frac{P_Y^2}{2M} + U(X) - U(Y) - \frac{\beta\Gamma^\downarrow\hbar}{4X_0M}G'\left(\frac{X-Y}{X_0}\right)(P_X - P_Y) + i\Gamma^\downarrow\left[G\left(\frac{X-Y}{X_0}\right) - 1\right] \right\} \rho(X, Y, t) \quad (2.12)$$

with an arbitrary initial condition

$$\rho(X, Y, 0) = \rho_0(X, Y). \quad (2.13)$$

This equation is the central object of our study and the remaining of the paper is devoted to determining various limiting regimes and the character of its solutions upon varying β , Γ^\downarrow , X_0 and \hbar . (In this paper we have already taken the limit $\kappa_0 \rightarrow \infty$.) At first glance the reader might get the impression that the slow subsystem we consider here is characterized by one degree of freedom only. As a simple analysis will show however that the slow subsystem can have an arbitrary number of degrees of freedom and most of the formulas we shall present are equally valid in this case.

This evolution equation is somewhat peculiar in certain aspects. It is obvious that in the absence of the coupling to the “reservoir”, it describes a purely quantum evolution of the “slow” subsystem. Eq. (2.12) has been derived from a purely quantum description of the entire system, by performing the expansion in β . In Eq. (2.12) however, the inverse temperature enters only in the combination $\tau_{th} = \beta\hbar$, which can be interpreted as a thermal time (analogous to the thermal de Broglie wave length). Thus the expansion in the inverse temperature β is at the same time an expansion in \hbar . Our limitation to the zeroth and first order terms in $\beta\hbar$ for the coupling between the “slow” subsystem and the “reservoir” can consequently be interpreted as a semiclassical approximation.

It has been argued by Diosi [4] that for the case of a Caldeira–Leggett correlator ($G(x) = 1 - x^2/2$) the similar high temperature limit of the evolution equation requires the retention of the next order term in β in order to bring the corresponding approximate evolution equation to a Lindblad form [13], which maintains positivity of the density distribution for any physically acceptable initial conditions. If these higher order terms in β are not introduced, such an equation (as Eq. (2.12)) cannot be applied to an initial state which is narrower than the thermal de Broglie wave length, $\lambda_T = 2\pi\hbar\sqrt{\beta/M}$. This restriction to wave packets which are wider than the thermal de Broglie wave length is manifest in a somewhat different way as well. Let us compute the rate of change of the “total energy” of the “slow” subsystem, which can be defined naturally as follows:

$$E_0(t) = \text{Tr}[H_0\rho(t)]. \quad (2.14)$$

Using the evolution equation Eq. (2.12) for the density matrix $\rho(X, Y, t)$, after some straightforward manipulations one obtains the following expression for the rate of change of the “total energy”:

$$\frac{dE_0(t)}{dt} = 2\gamma \left[\frac{T}{2} - \frac{\langle P^2 \rangle}{2M} \right], \quad (2.15)$$

where γ is the friction coefficient in the small velocity limit to be introduced below, see Eq. (3.2). This rate has an apparently pure classical content. This is of course deceiving, as quantum effects are clearly retained in both Eqs. (2.12) and (2.15), even though not entirely in Eq. (2.15). However, since one has to assume that $T > \hbar^2/ML^2$, where L is the characteristic spatial extension of the state, it is possible in Eq. (2.15) to replace the quantity $\langle P^2 \rangle = \langle P \rangle^2 + \langle\langle P^2 \rangle\rangle$ with simply $\langle P \rangle^2$. This renders Eq. (2.15) purely classical in character. One incurs a certain loss of accuracy and a small degree of inconsistency by proceeding in this manner, so it is better to leave Eq. (2.15) as is.

Even though one can go beyond the first order in β and one can derive a more accurate evolution equation for the density matrix $\rho(X, Y, t)$ in the high temperature limit, we shall not do that in this work, for the sake of simplicity of the presentation. We do not expect that such corrections will lead to a qualitatively new behaviour.

D. Coordinate and Momentum Distributions and the Cumulants Expansion

We will derive the time dependent solutions $\rho(X, Y, t)$ in the following sections, and from that it will be useful to extract information concerning the behavior of coordinates and momenta. The most convenient way to do so is through the cumulant expansion. To define this, we start by introducing the new variables:

$$r = \frac{X + Y}{2}, \quad s = X - Y. \quad (2.16)$$

Coordinate and momentum information can readily be extracted from the following rather atypical Fourier transform of the density matrix:

$$\rho(r, s, t) = \int \frac{dk}{2\pi\hbar} \exp\left(\frac{ikr}{\hbar}\right) d(s, k, t). \quad (2.17)$$

For either $s = 0$ or $k = 0$, $d(s, k, t)$ is the characteristic function [14] for the spatial or momentum distribution of a given quantum state respectively. For example, if we are interested in the spatial diffusion X , as measured by $\langle\langle X^2 \rangle\rangle$, then we get from Eq. (2.17) and integration by parts:

$$\langle X^2 \rangle = \int dX' \rho(X', X', t) X'^2 = -\hbar^2 \frac{d^2}{dk^2} d(0, k, t) |_{k=0} = \langle\langle X^2 \rangle\rangle + \langle X \rangle^2. \quad (2.18)$$

Similarly, in order to compute the average collective energy one needs $\langle P^2 \rangle$:

$$\begin{aligned}
\langle P^2 \rangle &= \int dX dX' \rho(X, X', t) \langle X' | P^2 | X \rangle \\
&= \frac{1}{2\pi\hbar} \int dX dX' dP \rho(X, X', t) \exp \left[\frac{iP(X' - X)}{\hbar} \right] P^2 \\
&= \int ds dP \exp \left(\frac{iPs}{\hbar} \right) d(s, 0, t) P^2 = -\hbar^2 \frac{d^2}{ds^2} d(s, 0, t) |_{s=0} = \langle\langle P^2 \rangle\rangle + \langle P \rangle^2.
\end{aligned} \tag{2.19}$$

The quantities denoted $\langle\langle \dots \rangle\rangle$ are the cumulants of the distribution.

From the definition of the function $d(s, k, t)$ one defines the general coordinate and momentum cumulant expansion as:

$$\ln d(s, k, t)|_{s=0} = \sum_{n=1}^{\infty} \frac{1}{n!} \left(\frac{ik}{\hbar} \right)^n \langle\langle r^n \rangle\rangle \tag{2.20}$$

$$\ln d(s, k, t)|_{k=0} = \sum_{n=1}^{\infty} \frac{1}{n!} \left(\frac{s}{i\hbar} \right)^n \langle\langle p^n \rangle\rangle \tag{2.21}$$

where $\langle\langle r^n \rangle\rangle$ and $\langle\langle p^n \rangle\rangle$ are the (time dependent) cumulants of the spatial and momentum distribution respectively. One can show that the zeroth order terms in both cumulant expansions vanish, which is consistent with the fact that the probability is conserved within the present formalism.

A Gaussian process has only non-vanishing first and second cumulants. In general it is known from Marcienkiewics' [17] or Pawula's [14] theorem, that for a probability distribution, one either has a Gaussian process with only the first two cumulants non-vanishing, or all cumulants are present. Furthermore, while there are some inequalities which relate cumulants of varying order, in most cases there is no restriction on their sign, which can be positive or negative.

E. Intrinsic States

By “integrating” over the intrinsic variables one of course loses a lot of information and only some average behavior of the slow subsystem can be thus inferred. In principle one can recover some of this information in the following manner. As in Refs. [6–9] one can introduce instead the generalized occupation number probabilities

$$\begin{aligned}
\mathcal{N}(X(t), Y(t), t, \varepsilon) &= \langle \phi | T_a \exp \left[\frac{i}{\hbar} \int_0^t dt'' H_1(Y(t'')) \right] | \varepsilon \rangle \\
&\times \langle \varepsilon | T \exp \left[-\frac{i}{\hbar} \int_0^t dt' H_1(X(t')) \right] | \phi \rangle
\end{aligned} \tag{2.22}$$

where $|\varepsilon\rangle$ is a “typical” state of the intrinsic subsystem with energy ε . One can derive now evolution equations for these quantities. With the help of these generalized occupation number probabilities one can introduce what was called in Refs. [8,9] the characteristic functional

$$\mathcal{N}(X(t), Y(t), t, \tau) = \int d\varepsilon \rho(\varepsilon) \mathcal{N}(X(t), Y(t), t, \varepsilon) \exp \left(\frac{i\varepsilon\tau}{\hbar} \right), \tag{2.23}$$

where $\rho(\varepsilon)$ is the average level density for the intrinsic subsystem. From this expression, by performing an inverse Fourier transform one can reconstruct the generalized occupation probabilities $\mathcal{N}(X(t), Y(t), t, \varepsilon)$. In such a case there is a double path integral representation for the density matrix for the slow subsystem with the condition that the intrinsic subsystem has a well defined energy ε , namely

$$\begin{aligned} \rho(X, Y, t, \varepsilon) = & \int dX_0 dY_0 \psi(X_0) \psi^*(Y_0) \int_{X(0)=X_0}^{X(t)=X} \mathcal{D}X(t) \int_{Y(0)=Y_0}^{Y(t)=Y} \mathcal{D}Y(t) \\ & \times \exp \left\{ \frac{i}{\hbar} [S_0(X(t)) - S_0(Y(t))] \right\} \rho(\varepsilon) \mathcal{N}(X(t), Y(t), t, \varepsilon). \end{aligned} \quad (2.24)$$

In principle this representation can be used to extract more detailed information concerning the time evolution of the coupled slow and complex intrinsic subsystems. We shall not attempt to do that however in this paper.

III. CLASSICAL LIMIT: KRAMERS EQUATION

It is interesting to explore the classical transport equation which emerges from Eq. (2.12). The standard approach is to construct the Wigner transform $f(Q, P, t)$ of the density matrix $\rho(X, Y, t)$ as

$$f(Q, P, t) = \frac{1}{2\pi\hbar} \int dR \exp \left(-\frac{iPR}{\hbar} \right) \rho \left(Q + \frac{1}{2}R, Q - \frac{1}{2}R, t \right). \quad (3.1)$$

It is well known that while $f(Q, P, t)$ can be interpreted as a classical probability distribution in a phase space (Q, P) , it is only a quasi-probability since its sign can be positive or negative at a given phase space point, while its integral over any unit phase space cell (of size \hbar) is positive semi-definite. We will further introduce the friction coefficient:

$$\gamma = \frac{\beta \Gamma^\downarrow \hbar}{2MX_0^2}. \quad (3.2)$$

As we will see, this definition will emerge naturally from our analysis of the dynamical evolution of the quantum systems. However, in taking the Wigner transform of $\rho(X, Y, t)$, we must also take the classical limits of the quantities Γ^\downarrow and X_0 , which have an intrinsic quantum interpretation. While it is not entirely clear to us how to define such limits, we will see that the combination which appears in γ has a natural classical interpretation.

From the definition, one can readily compute the classical evolution equation, which is simply the Wigner transform of the right hand side of (2.12):

$$\begin{aligned} \partial_t f(Q, P, t) = & \frac{1}{2\pi\hbar} \int dR \exp \left(-\frac{iPR}{\hbar} \right) \partial_t \rho \left(Q + \frac{1}{2}R, Q - \frac{1}{2}R, t \right) \\ = & \frac{1}{2i\pi\hbar^2} \int dR \exp \left(-\frac{iPR}{\hbar} \right) \left\{ -\frac{\hbar^2}{2M} \partial_Q \partial_R + U \left(Q + \frac{1}{2}R \right) - U \left(Q - \frac{1}{2}R \right) \right. \\ & \left. + i\Gamma^\downarrow \left[1 - G \left(\frac{R}{X_0} \right) \right] - i\gamma\hbar X_0 G' \left(\frac{R}{X_0} \right) \partial_R \right\} \rho \left(Q + \frac{1}{2}R, Q - \frac{1}{2}R, t \right) \end{aligned} \quad (3.3)$$

For the contribution due to the potential energy $U(X)$, one can use the Kramers–Moyal expansion

$$\begin{aligned} \int \frac{dR}{2\pi\hbar} \exp\left(-\frac{iPR}{\hbar}\right) \left[U\left(Q + \frac{1}{2}R\right) - U\left(Q - \frac{1}{2}R\right) \right] \rho\left(Q + \frac{1}{2}R, Q - \frac{1}{2}R, t\right) \\ = U(Q) \frac{2}{\hbar} \sin\left(\frac{\hbar \overleftarrow{\partial}_Q \overrightarrow{\partial}_P}{2}\right) f(Q, P, t) \\ = \partial_Q U(Q) \partial_P f(Q, P, t) + o(\hbar) \end{aligned} \quad (3.4)$$

where $\overleftarrow{\partial}_Q$ and $\overrightarrow{\partial}_P$ in the sine term act only on U and f , respectively. In the last line only terms to $o(\hbar)$ were retained. For the terms which depend upon the correlation function $G(x)$, we consider a general expansion

$$G(x) \approx 1 - \frac{x^2}{2} + \dots \quad (3.5)$$

The terms beyond the quadratic ones in the expansion will come with higher powers of \hbar into the evolution equation and are hence omitted. Integrating by parts and using the fact that $\rho(X, Y, t)$ vanishes when $X, Y \rightarrow \pm\infty$, we have:

$$\begin{aligned} \frac{\partial f(Q, V, t)}{\partial t} + V \frac{\partial f(Q, V, t)}{\partial Q} - \frac{1}{M} \frac{\partial U(Q)}{\partial Q} \frac{\partial f(Q, V, t)}{\partial V} \\ = \gamma \left\{ \frac{\partial [V f(Q, V, t)]}{\partial V} + \frac{T}{M} \frac{\partial^2 f(Q, V, t)}{\partial V^2} \right\}, \end{aligned} \quad (3.6)$$

where $T = 1/\beta$ is the temperature, and the velocity is $V = \dot{Q} = P/M$. We have thus obtained Kramers equation [14].

We will derive transport coefficients below, and it is worth noting that taking classical limits is not straightforward. In quantum Brownian motion, we will extract a diffusion constant which is related to the friction γ through the classical Einstein relation:

$$D = \frac{2X_0^2}{\beta^2 \Gamma \hbar} = \frac{T}{\gamma M}, \quad (3.7)$$

We note here that our transport theory has a consistent classical limit for all of these transport coefficients only when they remain finite as $\hbar \rightarrow 0$. This requires in turn that the parameters of our theory cannot remain constant as $\hbar \rightarrow 0$, if we are to recover a well defined classical transport.

IV. TIME DEPENDENT SOLUTIONS

In the remaining part of this article we will consider solutions to the evolution equations (2.12). For certain forms of the potential, one can readily obtain explicit solutions to the time evolution of the density matrix, while for others we solve the evolution equation numerically.

A. Exactly Solvable Limits

For the class of potentials:

$$U(X) = \begin{cases} -FX & \text{Section V} \\ \frac{1}{2}M\omega^2 X^2 & \text{Section VI} \\ -\frac{1}{2}M\Omega^2 X^2 & \text{Section VII} \end{cases} . \quad (4.1)$$

the evolution equation for the density matrix can be written as a first order partial differential equation in two variables, which is readily solved by the method of characteristics [15].

B. Numerical solutions

For other cases where one does not have analytic results, the method of solution can be chosen in many ways. For the double well potential, we have implemented two independent methods which agree. The first is a brute force technique in which we express the density matrix in the form

$$\rho(X, Y, t) = \sum_{n,m} \alpha_{nm}(t) \phi_m(X) \phi_n^*(Y) \exp \left[-\frac{i(E_m - E_n)t}{\hbar} \right], \quad (4.2)$$

where the $\phi(X)$ are the eigenstates in the absence of coupling to the intrinsic degrees of freedom:

$$H_0(X) \phi_n(X) = E_n \phi_n(X). \quad (4.3)$$

The evolution equations for $\alpha_{mn}(t)$ are solved numerically in a truncated N_{max}^2 dimensional basis, with $m, n = 1, \dots, N_{max}$. Typically we will use $N_{max} = 31$.

Alternatively, we have solved Eq. (2.12) on a two dimensional grid (X_k, Y_l) . It is found that the time iteration is most stable using the alternating-direction implicit method [16], with five points interpolation for the space derivatives. As a check on the validity of the solution, the total probability is verified to be preserved at unity:

$$\int dX \rho(X, X, t) = 1. \quad (4.4)$$

The latter method allows one to integrate much farther in time.

V. LINEAR POTENTIAL AND QUANTUM BROWNIAN MOTION

The classical picture of a Brownian particle in a constant force field F and interacting with a heat bath is described by the Langevin equation for the velocity:

$$\dot{v} + \gamma v - \frac{F}{M} = f(t) \quad (5.1)$$

Here γ is the friction coefficient, and $f(t)$ is Gaussian white noise. In the long time limit the particle energy equilibrates with $\langle\langle p^2 \rangle\rangle = TM$ and there is a finite drift velocity $v_\infty = F/\gamma M$.

In this section we consider the dynamics of a quantum particle in a constant force field interacting with our random matrix bath and contrast it to this classical limit. The results discussed here should be contrasted with those for the case $\beta = 0$, where we have found that the quantum dynamics is similar to turbulent diffusion [9,10].

A. Exact solution

Let us consider the case when there is a linear potential acting on the slow variables

$$H_0(X) = -\frac{\hbar^2}{2M}\partial_X^2 - FX. \quad (5.2)$$

One can consider the case of a time dependent linear potential as well, i.e. $U(X, t) = -F(t)X$, with only very slight modifications of the ensuing formulas. The equation for the density matrix now becomes

$$\left[i\hbar\partial_t + \frac{\hbar^2}{M}\partial_r\partial_s - \frac{i\beta\Gamma^\downarrow\hbar^2}{2X_0M}G'\left(\frac{s}{X_0}\right)\partial_s \right] \rho(r, s, t) = \{-Fs + i\Gamma^\downarrow[G(\frac{s}{X_0}) - 1]\}\rho(r, s, t) \quad (5.3)$$

with the initial condition $\rho(r, s, 0) = \rho_0(r, s)$. It is not necessary to consider a pure state as an initial state, and we allow for any general initial density matrix. The mixed partial derivative can be removed by passing to the Fourier transformed equation (see Section II.D) for $d(s, k, t)$. This satisfies the equation

$$\left\{ \partial_t + \left[\frac{k}{M} - \frac{\beta\Gamma^\downarrow\hbar}{2MX_0}G'\left(\frac{s}{X_0}\right) \right] \partial_s \right\} d(s, k, t) = \left\{ \frac{iFs}{\hbar} + \frac{\Gamma^\downarrow}{\hbar} \left[G\left(\frac{s}{X_0}\right) - 1 \right] \right\} d(s, k, t). \quad (5.4)$$

Using the method of characteristics for wave equations [15] one can find the solution in parametric form:

$$d(s, k, t) = d_0(S(t), k) \exp \left\{ \int_0^t dt' \left[\frac{iFS(t-t')}{\hbar} + \frac{\Gamma^\downarrow}{\hbar} \left[G\left(\frac{S(t-t')}{X_0}\right) - 1 \right] \right] \right\}, \quad (5.5)$$

$$\begin{aligned} \rho(r, s, t) &= \int \frac{dk}{2\pi\hbar} d_0(S(t), k) \\ &\times \exp \left\{ \int_0^t dt' \left[\frac{iFS(t-t')}{\hbar} + \frac{\Gamma^\downarrow}{\hbar} \left[G\left(\frac{S(t-t')}{X_0}\right) - 1 \right] \right] \right\}, \end{aligned} \quad (5.6)$$

where the time dependent function $S(t-t')$ is the solution of the auxiliary equation

$$\frac{dS(\tau)}{d\tau} = - \left[\frac{k}{M} - \frac{\beta\Gamma^\downarrow\hbar}{2MX_0}G'\left(\frac{S(\tau)}{X_0}\right) \right]. \quad (5.7)$$

Here $d(s, k, t)|_{t=0} = d_0(s, k)$ is the initial distribution, which is just the Fourier transform of $\rho_0(r, s)$. The coordinate s appears in this solution as an initial condition on S : $S(0) = s$. These equations define the flow of the density matrix in time. For an arbitrary t' the function $S(t-t')$ also satisfies the homogeneous equation

$$\left\{ \partial_t + \left[\frac{k}{M} - \frac{\beta \Gamma^\downarrow \hbar}{2X_0 M} G' \left(\frac{s}{X_0} \right) \right] \partial_s \right\} S(t - t') = 0. \quad (5.8)$$

Again, $S(t - t')$ depends on s through the initial condition. One can reexpress the full solution in terms of an initial density matrix ρ_0 as well:

$$\begin{aligned} \rho(r, s, t) = & \iint \frac{dr' dk}{2\pi \hbar} \rho_0(r', S(t)) \\ & \times \exp \left\{ \frac{ik(r - r')}{\hbar} + \int_0^t dt' \left[\frac{iFS(t - t')}{\hbar} + \frac{\Gamma^\downarrow}{\hbar} \left[G \left(\frac{S(t - t')}{X_0} \right) - 1 \right] \right] \right\}. \end{aligned} \quad (5.9)$$

There are no restrictions on the initial conditions $\rho_0(r, s)$, but it is convenient in our considerations below to use a particular form. If we have an initial Gaussian wavefunction, $\psi_0(X) = \exp(-X^2/4\sigma^2)/(2\pi\sigma^2)^{1/4}$, then:

$$\rho_0(r, s) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left(-\frac{4r^2 + s^2}{8\sigma^2} \right), \quad (5.10)$$

$$d_0(s, k) = \exp \left(-\frac{k^2 \sigma^2}{2\hbar^2} - \frac{s^2}{8\sigma^2} \right). \quad (5.11)$$

B. Attractors and Repellers

It is clear that the time evolution of $\rho(r, s, t)$ depends on the properties of $S(t)$. Hence the flow of the solution $\rho(r, s, t)$ can be better understood if we examine the stable and unstable fixed points of $S(t)$. In order to discuss further the character of this solution it is convenient to use a specific form for the correlator G , so for illustrative purposes we use $G(x) = \exp(-x^2/2)$. The fixed points are determined from the condition

$$k = \frac{\beta \Gamma^\downarrow \hbar}{2X_0} G' \left(\frac{s}{X_0} \right) \quad (5.12)$$

which is plotted in Fig. 1 (top). (The analogous result for the case of a periodic correlation function $G(x) = \cos[x]$ is shown in Fig. 1 (bottom).) This has a maximum value k_0 given by

$$k_0 = \frac{\beta \Gamma^\downarrow \hbar}{2\sqrt{e}X_0}. \quad (5.13)$$

The character of the trajectories $S(\tau)$ determined by solving Eq. (5.7) depends on whether $|k| > k_0$ or $|k| \leq k_0$. Since k is not dynamical, the evolution is only along the s direction. The flow lines $S(\tau)$ are shown in Fig. 1 with the arrows for selected values of k . As one can see, the part of the curve between $-1 < s/X_0 < 1$ is a line of stable fixed points (attractors), while for $|s/X_0| > 1$, it becomes a line of unstable fixed points (repellers). When $|k| > k_0$ the r.h.s. of Eq. (5.7) maintains a definite sign so $S(\tau)$ is either a monotonically increasing or decreasing function of time, for any given initial condition $S(0) = s$. When $-k_0 \leq k \leq k_0$ one

can see from Fig. 1 that there are two types of solutions. Furthermore, since k_0 depends on β , as $\beta \rightarrow 0$, $k_0 \rightarrow 0$ and the character of the dynamical evolution depends on temperature.

In general the trajectory $S(\tau)$ can be determined through a simple quadratures

$$\tau = \int_s^{S(\tau)} dx \left[-\frac{k}{M} + \frac{\beta \Gamma \downarrow \hbar}{2MX_0} G' \left(\frac{x}{X_0} \right) \right]^{-1}. \quad (5.14)$$

C. Momentum Cumulants – Thermalization

In order to determine the momentum cumulants we must construct the Taylor expansion of the function $\ln d(s, k, t)$ in powers of s at $k = 0$. One can see from Fig. 1 that along the $k = 0$ line, all trajectories flow to the origin $S = 0$ in the long time limit. By changing the integration variable in Eq. (5.5) from time to $x = s/X_0$, using Eq. (5.7), in the limit $t \rightarrow \infty$, where all trajectories have the property that $S(t) \rightarrow 0$ we obtain

$$\begin{aligned} \ln d(s, 0, t) &= \ln d_0(S(t), 0) + \frac{1}{i\hbar} \frac{2FMX_0^3}{\beta \Gamma \downarrow \hbar} \int_0^{s/X_0} dx \exp \left(\frac{x^2}{2} \right) \\ &+ \frac{2MX_0^2}{\hbar^2 \beta} \int_0^{s/X_0} \frac{dx}{x} \left[1 - \exp \left(\frac{x^2}{2} \right) \right]. \end{aligned} \quad (5.15)$$

From the power series expansion of the integrands, one can readily read off all the momentum cumulants in the limit $t \rightarrow \infty$. In this limit the initial condition become irrelevant as $\ln d_0(S(t), 0) \rightarrow 0$. In particular the first and second cumulants are:

$$\langle\langle p \rangle\rangle = \frac{2MF X_0^2}{\beta \Gamma \downarrow \hbar} = \frac{F}{\gamma} \quad (5.16)$$

$$\langle\langle p^2 \rangle\rangle = \frac{M}{\beta} = MT \quad (5.17)$$

One can see the physical picture emerging here. In the long time limit the quantum particle reaches a terminal velocity determined from the first cumulant:

$$v_\infty = \frac{\langle\langle p \rangle\rangle}{M} = \frac{2F X_0^2}{\beta \Gamma \downarrow \hbar} = \frac{F}{M\gamma}, \quad (5.18)$$

with the definition of the friction coefficient γ identical to that in the Kramers equation, Eq. (3.2). Furthermore, the kinetic energy of the particle equilibrates to the proper thermal equilibrium result:

$$\frac{\langle p^2 \rangle}{2M} = \frac{\langle\langle p \rangle\rangle^2}{2M} + \frac{\langle\langle p^2 \rangle\rangle}{2M} = \frac{Mv_\infty^2}{2} + \frac{T}{2}. \quad (5.19)$$

What is more notable, however, is that the momentum distribution has higher than second order cumulants, which increase exponentially with the order of the cumulant. In the absence of the linear potential ($F = 0$) only the even order cumulants are nonvanishing, and are given by:

$$\langle\langle p^{2n} \rangle\rangle = (-1)^{n-1} \frac{(2n-1)!!}{n} \frac{MX_0^2}{\hbar^2\beta} \left(\frac{\hbar}{X_0} \right)^{2n}. \quad (5.20)$$

The presence of F adds only odd cumulants:

$$\langle\langle p^{2n-1} \rangle\rangle = (-1)^{n-1} (2n-3)!! \frac{FX_0}{\gamma\hbar} \left(\frac{\hbar}{X_0} \right)^{2n-1}. \quad (5.21)$$

All higher than second order cumulants vanish in the strict classical limit $\hbar \rightarrow 0$. These cumulants also vanish in the limit $X_0 \rightarrow \infty$, which shall be interpreted as a weak coupling limit to the thermostat (which is the case in statistical physics). When the coupling to the “thermostat” is not weak, in the $t \rightarrow \infty$ limit the function $d(s, 0, t)$ (which is the Fourier transform of the momentum distribution) is narrower than a Gaussian and which thus leads to an equilibrium momentum distribution with longer tails. This is exemplified in Fig. 2, where we compare the natural logarithm of the momentum characteristic function Rel. (5.15) for the case when $M = \hbar = \beta = 1$, $F = 0$ with (from narrowest to widest) $X_0 = 0.1, 0.5, 1, 2$ and $X_0 = \infty$ (the Gaussian limit). The presence of a linear potential does not modify the absolute value of the characteristic function, only its phase.

Naively, one would have expected that the coupling to the thermostat is controlled by the magnitude of Γ^\downarrow alone. As one can easily convince oneself however, the coupling between the two systems is also controlled by the correlation length X_0 . In the limit $X_0 \rightarrow \infty$ there is no energy exchange between the two subsystems, irrespective of the value of the “coupling constant” Γ^\downarrow . For $X_0 = \infty$ the reservoir never responds to the “external agent” and only its excitation spectrum acquires GOE fluctuation characteristics if Γ^\downarrow , ρ_0 and κ_0 satisfy certain well known requirements.

D. Coordinate Cumulants and Diffusion

For the coordinate distributions, we compute the Fourier transform $d(s = 0, k, t)$. Since s enters as the initial condition, the solutions which characterize the spatial information are all trajectories with initial conditions $S(0) = s = 0$ and arbitrary k . From Fig. 1, we can see that there are three regions to consider: 1) for $|k| < k_0$ the trajectories have the property that $S(\tau \rightarrow \infty)$ approach the attractor exponentially, 2) for $|k| = k_0$, the trajectories approach the attractor as an inverse power law and 3) for $|k| > k_0$, the trajectories diverge linearly in time $S(\tau \rightarrow \infty) \rightarrow -\text{sign}(k) \infty$. We shall analyse next the behavior of the characteristic function $d(s = 0, k, t)$ in these different regimes.

1. $|k| < k_0$

For small k one can linearize Eq. (5.7) around the origin and solve the simpler equation:

$$\frac{dS(\tau)}{d\tau} = -\frac{k}{M} - \frac{\beta\Gamma^\downarrow\hbar S(\tau)}{2MX_0^2} = -\frac{k}{M} - \gamma S(\tau) \quad (5.22)$$

whose solution is

$$S(\tau) = \left(s + \frac{k}{\gamma M} \right) \exp(-\gamma\tau) - \frac{k}{\gamma M}. \quad (5.23)$$

In the $t \rightarrow \infty$ limit, by retaining only terms linear in time we obtain

$$\ln d(s, k, t)|_{s=0} = \ln d_0(S(t), k) + \frac{ik}{\hbar} \frac{2FX_0^2 t}{\beta\Gamma^\downarrow \hbar} - \frac{1}{2} \left(\frac{k}{\hbar} \right)^2 \frac{4\Gamma^\downarrow X_0^2 t}{(\beta\Gamma^\downarrow)^2 \hbar} + \mathcal{O}(k^3). \quad (5.24)$$

For an initial gaussian wavepacket, $\ln d_0(S(t), k) = -S^2(t)/8\sigma^2 - k^2\sigma^2/2\hbar^2$. In the long time limit, $S(t)$ approaches the fixed point $s_1(k)$ of (5.12), where $s_1(k) = -kM/\gamma + o(k^3)$. From this we can determine the first two spatial cumulants:

$$\langle\langle r \rangle\rangle = \frac{2FX_0^2}{\beta\Gamma^\downarrow \hbar} t = v_\infty t, \quad (5.25)$$

$$\langle\langle r^2 \rangle\rangle = \sigma^2 + \frac{\hbar^2}{4M^2\sigma^2\gamma^2} + \frac{4X_0^2}{\beta^2\Gamma^\downarrow \hbar} t = r_0^2 + 2Dt. \quad (5.26)$$

The constant term in $\langle\langle r^2 \rangle\rangle$ has two contributions. The first term is due to the initial width of the gaussian, while the second emerges in the long time limit, and is absent at $t = 0$. Physically we see a consistent picture of the quantum dynamics. The particle position grows linearly, with the velocity given by the terminal velocity obtained from $\langle\langle p \rangle\rangle$. Furthermore, the average position displays diffusion consistent with Brownian motion, which can be used to determine the diffusion constant D . This is the same expression for D as obtained from the fluctuation–dissipation theorem in the classical limit (Kramers equation) in Section III.

As with the momentum distribution, the coordinate distribution is not Gaussian, and has longer tails. (In the Brownian motion limit, these tails vanish; see below.) An analytical explicit construction of the entire spatial distribution and its cumulant expansion is not quite trivial, as the characteristic function $d(k, 0, t)$ has singularities and different asymptotic time behavior depending on the value of k . In particular, for small values of k the position of the repeller $s_2(k) \approx \text{sign}(k)X_0\sqrt{-2\ln|k|}$ is not analytical around $k = 0$. This is an indication that either various moments of the spatial distribution do not exist (perhaps they are divergent, as in the case of the Cauchy distribution) or they increase with time at a rate much faster than linear, similar to the case $\beta = 0$ discussed in Ref. [9]. In other words, the function $\ln d(s, k, t)|_{s=0}$ has some singularities in the k -plane, which have to be dealt with more carefully.

More generally, for $|k| < k_0$ and large times Eq. (5.7) can be written approximately as

$$\frac{dS(\tau)}{d\tau} = -\frac{\beta\Gamma^\downarrow \hbar}{2MX_0^2} \exp\left(-\frac{s_1(k)^2}{2X_0^2}\right) \left(1 - \frac{s_1(k)^2}{X_0^2}\right) (S(\tau) - s_1(k)), \quad (5.27)$$

where $s_1(k)$ is the k -dependent position of the attractor and the boundary condition is in this case $S(\tau \rightarrow \infty) \rightarrow s_1(k)$. In computing the leading term in t one can use this approximate trajectory. In this way one arrives at

$$\ln d(s, k, t)|_{s=0} \approx \ln d_0(s_1(k), k)|_{s=0} + \left\{ \frac{iFs_1(k)}{\hbar} + \frac{\Gamma^\downarrow}{\hbar} \left[\exp\left(-\frac{s_1(k)^2}{2X_0^2}\right) - 1 \right] \right\} t. \quad (5.28)$$

For small values of k the function $d(0, k, t)$ is narrower than a Gaussian, as one can establish easily by comparing the Taylor series in k of this expression with Eq. (5.24). Since the Fourier transform of this function is nothing else but the spatial distribution, we can thus conclude that at large distances the spatial distribution has longer tails than a Brownian particle.

2. $|k| = k_0$

For this critical value of k , the trajectory with initial condition $s = 0$, $k = \pm k_0$, will approach $S = \mp X_0$ in the limit $\tau \rightarrow \infty$, as seen in Fig. 1. It is sufficient to look at the case $k = k_0$. To examine the behavior of $S(\tau)$ in the neighborhood of the fixed point, it is convenient to take:

$$S(\tau) = -X_0(1 - \varepsilon(\tau)). \quad (5.29)$$

The dynamics is then given by

$$\frac{d\varepsilon(\tau)}{d\tau} = -\frac{k_0}{MX_0} + \gamma(1 - \varepsilon) \exp\left[-\frac{(1 - \varepsilon)^2}{2}\right] \simeq -\frac{k_0}{MX_0}\varepsilon^2. \quad (5.30)$$

The solution in terms of S then has the power-law behavior:

$$S(\tau) = -X_0 \frac{k_0 \tau}{k_0 \tau + MX_0}. \quad (5.31)$$

Substituting this into the solution for $d(s = 0, k, t)$, we obtain:

$$\begin{aligned} \ln d(0, k_0, t) = \ln d_0(S(t), k_0) + & \left[\left(\frac{k_0}{MX_0\gamma} - 1 \right) \frac{\Gamma^\downarrow}{\hbar} - i \frac{FX_0}{\hbar} \right] t \\ & + \left[\frac{\Gamma^\downarrow}{\hbar\gamma} + i \frac{FMX_0^2}{\hbar k_0} \right] \ln \left[1 + \frac{k_0}{MX_0} t \right] + o(k_0^3). \end{aligned} \quad (5.32)$$

3. $|k| > k_0$

In the other regime, when $|k| \gg k_0$ and $t \rightarrow \infty$, β no longer plays a role. Strictly speaking, this analysis is only valid in the $\beta = 0$ limit. The approximate equation for the trajectory is

$$\frac{dS(\tau)}{d\tau} = -\frac{k}{M}, \quad S(\tau) = -\frac{k}{M}\tau, \quad (5.33)$$

and thus the characteristic function acquires approximately the form

$$\ln d(s, k, t)|_{s=0} = \ln d_0\left(-\frac{kt}{M}, k\right) - \frac{iFkt^2}{2\hbar M} + \frac{\Gamma^\downarrow}{\hbar} \left[\frac{\sqrt{2\pi}MX_0}{2|k|} - t \right]. \quad (5.34)$$

Notice, that if for $|k| < k_0$ the characteristic function is narrower than a Gaussian, for $|k| > k_0$ one has just the opposite, the characteristic function tends to a time-dependent constant (*modulo* a nontrivial phase however). The above relation shows that the short distance behavior of the propagator has a quite unusual behavior. In order to construct the propagator one should use the initial density distribution $\rho_0(r, s) = \delta(r)$ and thus $d_0(s, k) = 1$). The above behaviour for large k implies that even at finite times an exponentially small part of the initial spatial distribution is left at the origin, namely $\exp(-\Gamma^\downarrow t/\hbar)\delta(r)$.

4. General Behavior for all k

An alternate manner to construct the coordinate distribution $d(0, k, t)$ is by solving numerically Eq. (5.7) for $S(t)$ and substituting the trajectory directly into Rel. (5.5) for $d(0, k, t)$. In Fig. 3 (top) we compare the numerical solution to Eqs. (5.5) and (5.7) (solid) with the Gaussian limit obtained by keeping only the second cumulant (dashes). The solutions are obtained for a time $t = 100$, and $X_0 = 1$. The results are all similar. However, if one goes to shorter correlation lengths, the importance of higher order cumulants is striking. In the bottom figure we show the same for a much shorter correlation length, $X_0 = 0.1$, also at $t = 100$. All the remaining parameters are kept at unity. As one can see, the exact result drops off abruptly at $k = k_0$. The reason is that for $|k| > k_0$, the function $S(t)$ escapes towards $-\infty$ linearly in time while the solution for $|k| \leq k_0$ slowly converges to the stable fixed points. If one factors out the overall $\exp(-\Gamma^\downarrow t/\hbar)$ from $|d(s, k, t)|$, the reminder grows exponentially in time for $|k| \leq k_0$ and tends to a time independent function for $|k| > k_0$ and as a result the discontinuity at $|k| = k_0$ becomes thus more pronounced.

E. Brownian Motion Limit

Even though we have shown that the system equilibrates to the correct thermal limit, the time evolution towards this equilibrium state is rather complex. For $k = 0$ all trajectories have the same asymptotic behaviour, $S(\tau \rightarrow \infty) \rightarrow 0$, irrespective of the initial conditions. It is not difficult however to see that if a trajectory starts far away from the origin, it will take an exponentially long time to reach the neighborhood of the origin, as the r.h.s. of Eq. (5.7) is exponentially small for $|s| \gg X_0$.

One can see from the expressions for the cumulants that if the limits (see also Ref. [9])

$$\frac{\hbar}{X_0} \rightarrow 0, \tag{5.35}$$

$$\frac{X_0}{\Gamma^\downarrow} \rightarrow 0 \tag{5.36}$$

are taken, with the friction coefficient γ remaining finite, one obtains the case of pure classical Brownian motion. All but the first two cumulants for coordinate and momenta vanish, and one is left with a Gaussian process. These limits can be achieved also by keeping \hbar finite and thus obtaining the case of a quantum Brownian particle.

VI. QUADRATIC POTENTIAL

A classical particle in a harmonic oscillator potential, treated with the Fokker–Planck or Langevin equations, will thermalize, with the equilibration given by the virial theorem. When the particle is quantum, the fluctuations are chaotic and moreover the coupling between the two subsystems is finite, we observe significant departures from the this idealized situation.

A. Exact Solution

For a particle in a harmonic oscillator potential, we start with

$$H_0(X) = -\frac{\hbar^2}{2M}\partial_X^2 + \frac{M\omega^2 X^2}{2}. \quad (6.1)$$

The equation for $d(s, k, t)$ can be solved through quadratures, in the same manner as for the linear potential. We note that the solution we obtain is not limited to the simple case under consideration. Analytic solutions are also possible if we want to include a linear time independent potential term, a general quadratic time dependent potential, and/or a multi-dimensional treatment.

We shall look for a solution using the same representation of the density matrix introduced in the previous Section in Rel. (2.17). The equation for density matrix is in this case

$$\begin{aligned} & \left[i\hbar\partial_t + \frac{\hbar^2}{M}\partial_r\partial_s - \frac{i\beta\Gamma^\downarrow\hbar^2}{2X_0M}G'\left(\frac{s}{X_0}\right)\partial_s - M\omega^2sr \right] \rho(r, s, t) \\ &= \left\{ i\Gamma^\downarrow \left[G\left(\frac{s}{X_0}\right) - 1 \right] \right\} \rho(r, s, t) \end{aligned} \quad (6.2)$$

and the corresponding equation for the function $d(s, t, k)$ is:

$$\left\{ \partial_t + \left[\frac{k}{M} - \frac{\beta\Gamma^\downarrow\hbar}{2MX_0}G'\left(\frac{s}{X_0}\right) \right] \partial_s - M\omega^2s\partial_k \right\} d(s, k, t) = \frac{\Gamma^\downarrow}{\hbar} \left[G\left(\frac{s}{X_0}\right) - 1 \right] d(s, k, t). \quad (6.3)$$

The solution of this equation can be obtained again using the method of characteristics [15]. In this case we will have a two-parameter solution for $d(s, k, t)$ which will depend on the functions $S(t)$ and $K(t)$ which satisfy the auxiliary equations:

$$\frac{dS(\tau)}{d\tau} = - \left[\frac{K(\tau)}{M} - \frac{\beta\Gamma^\downarrow\hbar}{2MX_0}G'\left(\frac{S(\tau)}{X_0}\right) \right], \quad (6.4)$$

$$\frac{dK(\tau)}{d\tau} = M\omega^2S(\tau) \quad (6.5)$$

with the initial conditions

$$S(\tau = 0) = s, \quad \text{and} \quad K(\tau = 0) = k. \quad (6.6)$$

We do not write the full solution here since it is more convenient to solve the equations in action–angle variables. Before we do so, let us examine the fixed point structure which will emerge.

B. Attractors and Repellers

The flow in the “phase space” (S, K) is not Hamiltonian in character, which is not surprising. Some typical trajectories are shown in Fig. 4 for $G(x) = \exp(-x^2/2)$. In this case there is no qualitative difference between the dynamics of this correlator or a periodic function such as $G(x) = \cos(x)$. In the top of Fig. 4 we have $\omega = 1$, $\gamma = 0.1$ while in the bottom the friction is stronger, with $\omega = 1$, $\gamma = 0.5$. The general pattern of the trajectories in the (S, K) -plane seems to be quite simple, in the limit $\tau \rightarrow \infty$, irrespective of the initial conditions, all trajectories spiral counterclockwise around the origin (unless the motion is overdamped). The origin is thus a stable focus. There are no trajectories going away to infinity in any direction in the “phase space” (S, K) . The plane (S, K) is separated into four regions by the two curves

$$S = 0 \quad \text{and} \quad \frac{K}{M} - \frac{\beta\Gamma^\dagger\hbar}{2MX_0}G'\left(\frac{S}{X_0}\right) = 0. \quad (6.7)$$

Each of these lines correspond to $\dot{K}(\tau) = 0$ and $\dot{S}(\tau) = 0$ respectively. Near the focus it is simpler to solve the linearized equations of motion

$$\frac{dS(\tau)}{d\tau} = -\frac{K(\tau)}{M} - \frac{\beta\Gamma^\dagger\hbar S(\tau)}{2MX_0^2}, \quad (6.8)$$

$$\frac{dK(\tau)}{d\tau} = M\omega^2 S(\tau), \quad (6.9)$$

which can be solved analytically. If the condition

$$\omega > \frac{\beta\Gamma^\dagger\hbar}{4MX_0^2} = \frac{\gamma}{2} \quad (6.10)$$

is fulfilled, then the required trajectories are

$$S(\tau) = \left[s \cos \bar{\omega}\tau - \frac{2k + M\gamma s}{2M\bar{\omega}} \sin \bar{\omega}\tau \right] \exp\left(-\frac{\gamma\tau}{2}\right), \quad (6.11)$$

$$K(\tau) = \left[k \cos \bar{\omega}\tau + \frac{\gamma k + 2M\omega^2 s}{2\bar{\omega}} \sin \bar{\omega}\tau \right] \exp\left(-\frac{\gamma\tau}{2}\right) \quad (6.12)$$

where

$$\bar{\omega} = \sqrt{\omega^2 - \left(\frac{\beta\Gamma^\dagger\hbar}{4MX_0^2}\right)^2} = \sqrt{\omega^2 - \frac{\gamma^2}{4}}, \quad (6.13)$$

The case $\omega < \gamma/2$ is formally similar to the case $\omega = i\Omega$ to be discussed in the next section. Strictly speaking, in the first order in β , in which we have derived our formulas so far, one has $\bar{\omega} \approx \omega$ and we shall use mostly this approximation from here on.

C. Solution in Action–Angle Coordinates

The flows shown in Fig. 4 suggest that action–angle coordinates might be better suited to the dynamical analysis of this problem. The analytical construction of the higher order cumulants is somewhat cumbersome and we shall limit our analysis to some general features. The action–angle variables are in this case

$$I = \frac{k^2}{2M\omega} + \frac{M\omega s^2}{2}, \quad (6.14)$$

$$\phi = \arctan \frac{k}{M\omega s}. \quad (6.15)$$

Here I is related to the energy. We can now rewrite the evolution equation Eq. (6.3) in these variables

$$\begin{aligned} \left\{ \partial_t - \omega \partial_\phi + \gamma \exp \left(-\frac{I \cos^2 \phi}{M\omega X_0^2} \right) \left[\sin \phi \cos \phi \partial_\phi + 2I \cos^2 \phi \partial_I \right] \right\} d(I, \phi, t) \\ = \frac{\Gamma^\downarrow}{\hbar} \left[\exp \left(-\frac{I \cos^2 \phi}{M\omega X_0^2} \right) - 1 \right] d(I, \phi, t). \end{aligned} \quad (6.16)$$

The equations for the trajectories acquire the following form

$$\frac{d\Phi(\tau)}{d\tau} = \omega - \frac{\gamma}{2} \sin 2\Phi(\tau) \exp \left\{ -\frac{I(\tau)}{2M\omega X_0^2} [1 + \cos 2\Phi(\tau)] \right\}, \quad (6.17)$$

$$\frac{dI(\tau)}{d\tau} = -\gamma I(\tau) [1 + \cos 2\Phi(\tau)] \exp \left\{ -\frac{I(\tau)}{2M\omega X_0^2} [1 + \cos 2\Phi(\tau)] \right\} \quad (6.18)$$

with initial conditions

$$I(0) = \frac{k^2}{2M\omega} + \frac{M\omega s^2}{2}, \quad (6.19)$$

$$\Phi(0) = \arctan \frac{k}{M\omega s}. \quad (6.20)$$

Irrespective of the initial conditions the action $I(\tau)$ is always a monotonically decreasing function, vanishing in the long time limit. If the motion is not overdamped (i.e. $\omega > \gamma/2$) the phase $\Phi(\tau)$ is a monotonically increasing function of time. In the weak friction limit, when $\gamma \ll \omega$, one can replace the equations for the trajectories with the following approximate equations

$$\frac{d\Phi(\tau)}{d\tau} = \omega, \quad (6.21)$$

$$\frac{dI(\tau)}{d\tau} = -\gamma I(\tau) \exp \left[-\frac{I(\tau)}{2M\omega X_0^2} \right] \left[\mathcal{I}_0 \left(\frac{I(\tau)}{2M\omega X_0^2} \right) - \mathcal{I}_1 \left(\frac{I(\tau)}{2M\omega X_0^2} \right) \right], \quad (6.22)$$

obtained after averaging the initial equations over the fast motion (i.e. over one period $2\pi/\omega$). Here $\mathcal{I}_0(x)$ and $\mathcal{I}_1(x)$ are the modified Bessel functions of first kind. The r.h.s. of

Eq. (6.22) behaves linearly in I for small values of the action and as $1/\sqrt{I}$ for large values. This behaviour is consistent with the fact that the friction term is effective only near the origin in coordinate, i.e. for $s \approx \mathcal{O}(X_0)$.

After manipulations similar to those used in the previous section, and averaging over the fast motion and by changing the integration variable from time to action (using Eq. (6.22)), one obtains that the asymptotic expression for the characteristic function is

$$\ln d(I, \phi, t) = \frac{2MX_0^2}{\hbar^2\beta} \int_0^I \frac{d\alpha}{\alpha} \left[\mathcal{I}_0 \left(\frac{\alpha}{2M\omega X_0^2} \right) - \exp \left(\frac{\alpha}{2M\omega X_0^2} \right) \right] \times \left[\mathcal{I}_0 \left(\frac{\alpha}{2M\omega X_0^2} \right) - \mathcal{I}_1 \left(\frac{\alpha}{2M\omega X_0^2} \right) \right]^{-1} \quad (6.23)$$

where $I = I(0)$, which was defined above as the initial value of the action variable. One can construct in a straightforward manner all the spatial and momentum cumulants, by reverting to the initial space-momentum variables s and k . Note that $d(s, k, t) = d(I, \phi, t)$ is time independent in this limit, as expected. One can extract easily the behaviour for large and small I .

$$\ln d(I, \phi, t) \approx \begin{cases} -\frac{I}{\hbar^2\omega\beta} - \frac{3I^2}{16\hbar^2\beta\omega^2MX_0^2} & I \ll M\omega X_0^2, \\ -\frac{8\sqrt{2\pi}MX_0^2}{3\beta\hbar^2} \left[\frac{I}{2M\omega X_0^2} \right]^{3/2} & I \gg M\omega X_0^2. \end{cases} \quad (6.24)$$

By taking the Fourier transform of the above expression for $d(s, k, t)$ for either $k = 0$ or $s = 0$ one can determine either the momentum or the spatial equilibrium distribution of a harmonic oscillator coupled with a “reservoir”. For the oscillator, the action variable I is, up to a trivial factor, simply the total energy E . Hence one can also extract the energy distribution from the above expressions.

D. Eigenvalues of the Time Evolution Operator

It is instructive to construct the eigenvalues and the eigenvectors of the time evolution operator. If we rewrite the time evolution equation for the density matrix in the form,

$$i\hbar\partial_t\rho(r, s, t) = \mathcal{O}\rho(r, s, t) \quad (6.25)$$

we can consider the eigenvalue problem associated with \mathcal{O} :

$$\mathcal{O}\rho(r, s) = \lambda\rho(r, s). \quad (6.26)$$

The equilibrium solution will correspond to $\lambda = 0$, and in general the spectrum should be complex. While an analytical solution does not seem possible for a general $G(x)$, if we take $G(x) = 1 - x^2/2$, one can readily solve the problem.

For the equilibrium state ($\lambda = 0$) one obtains

$$\rho_0(r, s) = \exp \left\{ -\frac{\beta M\omega^2 r^2}{2} - \frac{M}{2\beta\hbar^2} s^2 \right\}. \quad (6.27)$$

We will discuss the physical properties of this solution in the next section. This problem now becomes identical to the eigensolutions of the Fokker–Planck equation for the oscillator [14]. Following that analysis, the eigenvalue spectrum is given in terms of two integers, n_1 and n_2 . The basic roots are

$$\lambda_{\pm} = -\frac{i\gamma\hbar}{2} \pm \hbar\bar{\omega}, \quad \bar{\omega} = \sqrt{\omega^2 - \frac{\gamma^2}{4}} \quad (6.28)$$

and the entire spectrum can be written as:

$$\lambda_{n_1, n_2} = -\frac{i\gamma\hbar}{2}(n_1 + n_2) + \hbar\bar{\omega}(n_1 - n_2), \quad (n_i = 0, 1, \dots) \quad (6.29)$$

The time evolution of the density matrix will equilibrate to the $\lambda = 0$ eigenvector, as all other components will decay in time as $\exp[-(n_1 + n_2)\gamma t/2\hbar]$. The temperature dependence appears indirectly through γ , which vanishes in the $\beta = 0$ limit. These patterns are shown in Fig. 5 for $\beta > 0$, where it is clear that all eigenvalues with the exception of the equilibrium state ($\lambda = 0$) lead to decay. For $\beta = 0$, the spectrum collapses to the real axis, and all points $\lambda = n\bar{\omega}$ are infinitely degenerate.

E. Recovery of Equilibrium Thermodynamics

For the harmonic oscillator, we would like to see whether or not the random matrix bath can act as an ideal heat bath. The quantum equilibrium density matrix we would expect is:

$$\rho_{eq}(X, Y) = \sum_{n=0}^{\infty} \exp\left[-\beta\left(n + \frac{1}{2}\right)\hbar\omega\right] \phi_n(X)\phi_n(Y) \quad (6.30)$$

where ϕ_n are the oscillator wavefunctions given by:

$$\phi_n(X) = \left[\frac{\alpha^2}{\pi 2^{2n}(n!)^2}\right]^{1/4} H_n(\alpha X) \exp\left(-\frac{\alpha^2 X^2}{2}\right), \quad \alpha^2 = \frac{M\omega}{\hbar}. \quad (6.31)$$

and H_n is the Hermite polynomial. Defining $z = \exp[-\beta\hbar\omega]$, we can write:

$$\rho_{eq}(X, Y) = \sqrt{\frac{\alpha z}{\pi}} \exp\left[-\frac{\alpha^2(X^2 + Y^2)}{2}\right] \sum_{n=0}^{\infty} \left(\frac{z}{2}\right)^n \frac{1}{n!} H_n(\alpha X) H_n(\alpha Y) \quad (6.32)$$

$$= \sqrt{\frac{\alpha z}{\pi(1 - z^2)}} \exp\left\{-\frac{\alpha^2}{2(1 - z^2)} [(X^2 + Y^2)(1 + z^2) - 4XYz]\right\} \quad (6.33)$$

In the last line we have used the generating function for Hermite polynomials. If we take the leading order in β and transform from X, Y to r, s , we find

$$\rho_{eq}(r, s) \simeq \sqrt{\frac{\alpha}{2\pi\beta\hbar}} \exp\left[-\frac{\alpha^2}{2\beta\hbar\omega} s^2 - \frac{\alpha^2\beta\hbar\omega}{2} r^2\right], \quad (6.34)$$

which is precisely the $\lambda = 0$ eigenvector found in the previous section. Hence, to leading order in β (and \hbar in a sense, as β enters as $\beta\hbar$), and in the Brownian Motion limit, we recover the equilibrium density matrix. In general the equilibrium density matrix will have a non-Gaussian character.

F. Cumulant Expansion

To get the cumulants, one can use the procedure described previously (see also Ref. [9]) and derive that in the $t \rightarrow \infty$ limit

$$\frac{\langle\langle p^2 \rangle\rangle}{2M} = \frac{\langle\langle M\omega^2 r^2 \rangle\rangle}{2} = \frac{1}{2\beta} = \frac{T}{2}, \quad (6.35)$$

as one might have expected. The higher order cumulants can be obtained by setting $k = 0$ or $s = 0$ respectively in the Taylor expansion in I of the Rel. (6.23). We shall not try here to derive explicit expressions for higher order cumulants, as they apparently seem to be quite complicated and hardly very revealing. As Rel. (6.24) clearly shows, the equilibrium distribution is much narrower than a Gaussian one, which is already indicative of the presence of nonnegligible higher than second order cumulants. In Fig. 6 we compare $\ln d(I, \phi, t \rightarrow \infty)$ as a function of \sqrt{I} obtained from Eq. (6.23) for $X_0 = 0.5, 1, 2, \infty$ (narrowest to widest). The widest $X_0 = \infty$ is the equilibrium distribution $\exp(-\beta H_0)$, (the first term in the low I expansion, see Rel. (6.24)). Notice that the equilibrium distribution is independent of ϕ as well as of the actual values of the friction coefficient γ and of the coupling constant Γ^\downarrow . Except for a “trivial” overall factor, the shape of this function is controlled by a single parameter, the “characteristic action” $2M\omega X_0^2$, which depends on the “roughness” of the coupling to the “reservoir”.

VII. INVERTED PARABOLIC POTENTIAL

The tunneling through a potential having the shape of an inverted parabola can be studied by performing the formal replacement $\omega = i\Omega_0$ in the corresponding equations of the previous section.

A. Fixed Points

The equations for the trajectories $(S(\tau), K(\tau))$ become now

$$\frac{dS(\tau)}{d\tau} = - \left[\frac{K(\tau)}{M} - \frac{\beta\Gamma^\downarrow\hbar}{2MX_0} G' \left(\frac{S(\tau)}{X_0} \right) \right], \quad (7.1)$$

$$\frac{dK(\tau)}{d\tau} = -M\Omega_0^2 S(\tau). \quad (7.2)$$

The two curves we have introduced in the previous section

$$S = 0 \quad \text{and} \quad \frac{K}{M} - \frac{\beta\Gamma^\downarrow\hbar}{2MX_0} G' \left(\frac{S}{X_0} \right) = 0, \quad (7.3)$$

play a similar role in this case as well. However, the general flow pattern in the “phase space” (S, K) has an entirely different aspect, as shown in Fig. 7. The origin is now an unstable focus point. Near the origin we can again use the linear approximation $G'(x) \approx -x$ and thus consider the much simpler equations

$$\frac{dS(\tau)}{d\tau} = -\frac{K(\tau)}{M} - \frac{\beta\Gamma\hbar S(\tau)}{2MX_0^2}, \quad (7.4)$$

$$\frac{dK(\tau)}{d\tau} = -M\Omega_0^2 S(\tau). \quad (7.5)$$

The imaginary eigenfrequencies are

$$\Omega_{\pm} = -\frac{\gamma}{2} \pm \sqrt{\Omega_0^2 + \frac{\gamma^2}{4}} = -\frac{\gamma}{2} \pm \Omega \quad (7.6)$$

with $\Omega_+ \geq 0$ and $\Omega_- < 0$. One can easily recognize that Ω_+ is the renormalized attempt frequency in the classical Kramers result for the transmission through a barrier [3].

As we have noted in the previous section the case of an inverted parabolic potential bears some formal similarities with the case of over damped motion ($\omega < \gamma/2$), with only one difference, that both imaginary eigenfrequencies are negative. We shall not discuss this case in detail in this paper.

For arbitrary initial conditions $S(0) = s$, $K(0) = k$ in the neighborhood of the origin almost all trajectories are diverging exponentially away as $\exp(\Omega_+\tau)$, except when s and k are exactly along the line

$$k = \left(1 - \frac{\gamma}{2\Omega}\right) M\Omega s. \quad (7.7)$$

For sufficiently large s the stable manifold is defined by the line

$$k = M\Omega_0 s. \quad (7.8)$$

For small friction coefficient ($\gamma \ll \Omega_0$) these two lines are almost identical. For large values of the friction coefficient however ($\gamma \gg \Omega_0$) the stable manifold near the origin almost coincides with the Os -axis.

The solution to the above linearized equations of motion are

$$S(\tau) = \left[\frac{s}{2} \left(1 - \frac{\gamma}{2\Omega}\right) - \frac{k}{2M\Omega} \right] \exp \left[\left(\Omega - \frac{\gamma}{2} \right) \tau \right] + \left[\frac{s}{2} \left(1 + \frac{\gamma}{2\Omega}\right) + \frac{k}{2M\Omega} \right] \exp \left[- \left(\Omega + \frac{\gamma}{2} \right) \tau \right], \quad (7.9)$$

$$K(\tau) = \left[\frac{k}{2} \left(1 + \frac{\gamma}{2\Omega}\right) - \frac{M\Omega_0^2 s}{2\Omega} \right] \exp \left[\left(\Omega - \frac{\gamma}{2} \right) \tau \right] + \left[\frac{k}{2} \left(1 - \frac{\gamma}{2\Omega}\right) + \frac{M\Omega_0^2 s}{2\Omega} \right] \exp \left[- \left(\Omega + \frac{\gamma}{2} \right) \tau \right]. \quad (7.10)$$

With increasing time and for initial conditions such that $|S(0) = s| \gg X_0$, the term responsible for friction in Eqs. (7.2) becomes negligible and the trajectories are governed by exponentials $\exp(\pm\Omega_0\tau)$.

In the case of very small friction ($\gamma \ll \Omega_0$) one can obtain an approximate expression for the trajectory $S(\tau)$. If one is interested in the character of the spatial distribution and

the way this is modified in the presence of dissipation, one needs trajectories with initial conditions $S(0) = 0$, $K(0) = k$ only, namely

$$S(\tau) = -\frac{k \sinh \Omega_0 \tau}{M \Omega_0} \exp \left[-\int_0^\tau d\tau' \frac{\tilde{\gamma}(\tau')}{2} \right], \quad (7.11)$$

$$K(\tau) = \left[k \cosh \Omega_0 \tau + \frac{k \tilde{\gamma}(\tau) \sinh \Omega_0 \tau}{2 \Omega_0} \right] \exp \left[-\int_0^\tau d\tau' \frac{\tilde{\gamma}(\tau')}{2} \right], \quad (7.12)$$

where the “instantaneous” friction coefficient is defined as follows

$$\tilde{\gamma}(\tau) = \gamma \exp \left(-\frac{k^2 \sinh^2 \Omega_0 \tau}{2 M^2 \Omega_0^2 X_0^2} \right). \quad (7.13)$$

Using these expressions one obtains for the characteristic function for the spatial distribution the following expression

$$d(0, k, t) = d_0(S(t), K(t)) \exp \left\{ -\frac{\Gamma^\downarrow}{\hbar} \int_0^t d\tau \left[\exp \left(-\frac{S^2(\tau)}{2 X_0^2} \right) - 1 \right] \right\}. \quad (7.14)$$

In spite of the fact that it is hopeless to evaluate analytically this expression as a function of k and time t (there are at least five exponentials nested into one another), even a cursory analysis of the k -dependence originating from dissipation alone shows that this function is significantly narrower than a Gaussian. This at once is indicative of the presence of higher than second order cumulants in the spatial distribution, but most of all of the fact that the spatial distribution has a wider spread than the corresponding one obtained in traditional approaches. If one were to perform a Taylor expansion of the integrand in powers of k to determine the cumulants for example, one observes that each power of k is always multiplied by $\sinh \Omega_0 \tau$. Upon performing the time integral one thus obtains that all cumulants increase exponentially with time and that in particular all of them are positive as well.

B. Eigenvalues

The eigenvalues of the evolution equation are obtained from those of the harmonic oscillator, by making the transformation $\omega = i\Omega_0$. Again, specializing to the case $G(x) = 1 - x^2/2$, we obtain the spectrum:

$$\lambda_\pm = -i\hbar \left[\frac{\gamma}{2} \pm \sqrt{\Omega_0^2 + \frac{\gamma^2}{4}} \right] = i\hbar \Omega_\mp, \quad (7.15)$$

$$\lambda_{n_1, n_2} = -\frac{i\gamma\hbar}{2}(n_1 + n_2) + i\hbar \sqrt{\Omega_0^2 + \frac{\gamma^2}{4}}(n_1 - n_2), \quad (n_i = 1, 2, \dots)$$

In this case the eigenvalue $\lambda = 0$, which corresponds to an equilibrium solution, is no longer present. The eigenvalues are all purely imaginary, and have values above and below the real axis. The occurrence of eigenvalues with positive imaginary parts is due to the unphysical asymptotic behaviour of an inverted parabola potential, and thus to the absence of an equilibrium distribution.

C. Remarks on Tunneling

Kramers showed that dissipation leads to a reduction of the flux through an inverted parabolic barrier, as the unperturbed attempt frequency in the transition state theory should be replaced with the renormalized one $\Omega_0 \rightarrow \Omega_+ \leq \Omega_0$ [3]. One basic assumption in Kramers approach was the fact that the friction coefficient is momentum independent. The present approach can be interpreted as a theory with a momentum dependent friction coefficient, which in the zero velocity limit reduces to the classical value. For finite velocities however, the effective friction coefficient in our approach is smaller than the one for zero velocity (see the above approximate solution for the trajectory for the case of small friction). One can thus expect two effects: *i*) the effective or average attempt frequency in our approach is in between the Kramers value and the value corresponding to no friction, i.e. $\Omega_+ < \Omega_{eff} < \Omega_0$; *ii*) the spatial density distribution is also modified. Unfortunately the rest of our argument concerning the behaviour of the spatial distribution is pure qualitative at the present time. In the classical transition theory the flux through the barrier is controlled by the probability population of the states at the top of the barrier. With decreasing friction coefficient, the thermalization of the spatial distribution in the classically allowed region is less effective and as a result the overall flux through the barrier decreases as well. In the previous section we have established that the energy distribution has generally wider tails than a pure Boltzmann distribution and thus states with higher energies have a higher relative probability to be populated when the coupling strength between the “reservoir” and the subsystem is finite. It is thus reasonable to expect that tunneling states would have a higher relative occupation probability in our approach. Overall the effect of an effective momentum dependent friction coefficient is likely to lead to an enhancement of the tunneling probability when compared with the classical Kramers result. Since the role of the pure quantum effects and the role of the finite coupling strength to the “reservoir” are intimately related, we cannot at the present time disentangle the specific role played by each one of them separately.

VIII. TUNNELING IN A DOUBLE WELL POTENTIAL

For the problem of tunneling, we consider also the dynamical evolution of a particle in the double well potential given by:

$$H_0(X) = -\frac{\hbar^2}{2M}\partial_X^2 + a\left(X^2 - \frac{b}{2a}\right)^2. \quad (8.1)$$

For this or more complex potentials, analytic solutions are no longer possible. The form of the potential is shown in Fig. 8, together with the first few eigenvalues corresponding to the parameters $a = 5$, $b = M = 1/2$.

A. Tunneling Rates

The numerical solution of the evolution Eq. (2.12) for the density matrix is done as explained in Sect. IV.B. Let us examine first the effect of dissipation on tunneling. For this

purpose, we first put $\beta = 0$ and solve the equation for some representative values of the parameter Γ^\downarrow . Let $\phi_1(X)$ and $\phi_2(X)$ be the first two eigenstates of the double well. We take as initial state the combination

$$\phi_0(X) = \frac{1}{\sqrt{2}}[\phi_1(X) - \phi_2(X)], \quad (8.2)$$

which represents a wave packet that is mostly localized in the left well of Fig. 8. In view of the fact that splitting between the first two states is very small, $\Delta E \approx 3 \times 10^{-6}$, the tunneling of the wave packet to the other well would take a very long time should there be no dissipation. Fig. 9 shows the strength that tunnels through the barrier as function of the time for some values of Γ^\downarrow . At the beginning of the tunneling process, the rate increases almost linearly with this parameter. For very large time, all the tunneled strengths approach the limiting value $1/2$ corresponding to the equal distribution between the two wells.

B. Temperature Dependence

Next, we study the dependence of the tunneling on the temperature. For this, we fix a value of Γ^\downarrow and solve the evolution equation for different values of β . One would expect that the rate would increase with the temperature, i.e. when β decreases. Fig. 10 shows such a behaviour for five values of $\beta = 0., 0.05, 0.10, 0.15, 0.20$. For larger values of β , the strength on the right hand side may come out negative for reasons we discussed in Sect. II.

C. Comparison to the Caldeira–Leggett Approach

At this point, we are also able to compare our results with that obtained from the Caldeira–Leggett model. To reproduce the latter, it is sufficient to replace the Gaussian form of the correlation function that we have used up to now by its quadratic approximation $G(x) = 1 - x^2/2$. The effect may be seen better by choosing a smaller value for the correlation length X_0 . Fig. 11 shows the density distribution after the time $t = 4$ for the parameters $X_0 = 0.2$, $\beta = 0$, $\Gamma^\downarrow = 1$. The difference is quite appreciable (notice the ordinate logscale), not only in the tunneled strengths but also in their shapes.

D. Eigenvalues of the Evolution Operator

We have numerically computed the eigenvalue spectrum by expanding the density matrix in the eigenvectors of this quartic potential. Taking $N_{max} = 31$, we have diagonalized the evolution operator \mathcal{O} . The complex eigenvalues with the smallest imaginary parts are shown in Fig. 12 (top) for $\beta = 0$ and 0.2 . If we denote the eigenvectors as $\rho_k(X, Y)$, then the time evolution, which includes the tunneling, has the form

$$\rho(X, Y, t) = \sum_k \alpha_k \exp\left(-\frac{i\lambda_k t}{\hbar}\right) \rho_k(X, Y). \quad (8.3)$$

One can see in Fig. 12 that the tunneling can be influenced by several nearby eigenvalues, and that as β increases, the patterns of important eigenvalues changes considerably. In the bottom of Fig. 12, we plot the imaginary parts of the eigenvalues as a function of temperature for the ones with the smallest imaginary component. One observes that the imaginary part of the eigenvalue with the smallest nonvanishing absolute value apparently vanishes in the limit $T \rightarrow 0$. This is consistent with Caldeira and Leggett’s conclusion [2] that at $T = 0$ dissipation decreases the tunnelling rate. This is not true however at high temperatures, as one can see.

IX. CONCLUDING REMARKS

We have developed a dynamical theory of simple quantum systems coupled to complex quantum environments, where the environment is a general “chaotic” bath of intrinsic excitations. The model Hamiltonian we introduce for the intrinsic subsystem incorporates the generic properties of finite many-body systems. This includes an average level density of states sharply increasing with energy, the presence of universal spectral (or random matrix) fluctuations for the intrinsic system and the variation of these properties while changing the “shape” of the intrinsic system modeled with parametric banded random matrices. In this way, the intrinsic system is capable to easily absorb energy due to its large heat capacity. We did not yet allow the intrinsic system to perform mechanical work, but this feature can be readily implemented.

We are able to solve the dynamical evolution equations for these systems, without making any uncontrollable approximations or assumptions. Using the Feynman–Vernon path integral approach, we derive the random matrix influence functional, and an evolution equation for the density matrix of the “slow” subsystem at finite, but high temperatures. This evolution equation is surprisingly easy to manipulate and in many instances one can construct full solutions by quadratures, for cases when the corresponding path integral can be computed only by brute force. The entire treatment is performed at the quantum level. We have shown on the other hand that in the classical limit, the evolution equation reduces to the Kramers form.

Our analysis was limited to the case when the motion of the simple system can be treated in the adiabatic approximation. Thus, we have not taken advantage of another parameter in our description of the reservoir, the bandwidth of the random matrix κ_0 . It is well known that banded random matrices lead to localization [18]. It would be very interesting to explore whether localization in the “reservoir” states induces localization in the simple quantum system coupled to such a reservoir. (One can show that for finite bandwidths κ_0 the influence functional in our model can be brought to a form similar to the one suggested by Cohen [11] to describe localization, although we did not analyze this limit here.)

The quantum evolution equation we have derived for the density matrix is not more complicated than a classical Fokker–Planck equation. However, this evolution equation describes processes which first of all are quantum in nature and moreover have manifestly non-Gaussian features. So although we started with a Gaussian process characterized by our parametric random matrices, we ended up with a non-Gaussian dynamical process. Unlike traditional approaches, we have not assumed that the coupling to the “reservoir” is

vanishingly small. In particular, this is one of the reasons why the diffusion process acquires a non-Gaussian character. The spatial and momentum distributions are characterized by high order cumulants, which increase exponentially with the order. As we have discussed earlier [9], this is indicative of the fact that the corresponding distributions have longer tails than previously expected. In order to put in evidence such features, one ought to be careful about the order in which the various limits are taken. If one takes the semiclassical limit first in the evolution equation for the density matrix, such features are lost. If in the actual quantum solution one takes either the semiclassical limit ($\hbar \rightarrow 0$) or the limit of weak coupling to the reservoir (either $\Gamma^\downarrow \rightarrow 0$ or/and $X_0 \rightarrow \infty$) then one recovers the standard results as well. We have thus shown that, at least in the framework of the present model (which we believe to be sufficiently generic), both semiclassical and weak coupling limits have a rather singular character, which is seen in the temporal domain or/and the phase space distributions.

The particular form of the quantum evolution equation we have discussed in this paper has one rather unnecessary restriction, based on the “translational invariant” form of the influence functional we have used, see Eq. (2.11), which lead to Eq. (2.12). One can easily convince oneself that this form we have assumed can be easily amended and, to within some approximation, a more general quantum evolution equation for the density matrix of the “slow” subsystem can be derived, namely:

$$i\hbar\partial_t\rho(X,Y,t) = \left\{ \frac{P_X^2}{2M} - \frac{P_Y^2}{2M} + U(X) - U(Y) - \frac{\gamma X_0^2}{2} \frac{\partial G(X,Y)}{\partial s} [P_X - P_Y] + i\Gamma^\downarrow [G(X,Y) - 1] \right\} \rho(X,Y,t) \quad (9.1)$$

where $s = X - Y$ and where the correlator $G(X,Y)$ satisfies the only symmetry requirements $G(X,Y) = G(Y,X) = G^*(X,Y)$. One has to interpret γ , β , Γ^\downarrow and $G(X,Y)$ as phenomenological quantities, characterizing the “reservoir” and its coupling to the “slow” subsystem. We thus have now at our disposal a quantum evolution equation, with an effective velocity dependent friction coefficient, a finite coupling strength to the “reservoir” and which in the classical and weak coupling limits reduces to the Kramers equation. In the weak coupling limit only this evolution equation is equivalent to the high temperature limit of the Caldeira–Leggett model.

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APPENDIX A: EVOLUTION EQUATIONS FOR THE AVERAGE PROPAGATOR AND THE INFLUENCE FUNCTIONAL

The time evolution of the fast subsystem is found by solving the time-dependent Schrödinger equation in the form [6–10]:

$$\phi(t) = T \exp \left[-\frac{i}{\hbar} \int_0^t ds H_1(X(s)) \right] \phi(0) = \mathcal{U}(X(t)) \phi(0). \quad (\text{A1})$$

where T is the time ordering operator, and $\mathcal{U}(X(t))$ the propagator. (We assume that the initial state $\phi(0)$ is uncorrelated with the Hamiltonian $H_1(X(t))$ at later times; correlated initial conditions have been discussed elsewhere [6].) One can show that in the leading order in an expansion in $1/N_0$ the average propagator $U(X(t)) = \overline{\mathcal{U}(X(t))}$ is diagonal in the representation we have chosen. Its diagonal matrix elements have the following form

$$U_k(X(t)) = \overline{\langle k | T \exp \left[-\frac{i}{\hbar} \int_0^t ds H_1(X(s)) \right] | k \rangle} = \exp \left(-\frac{i\varepsilon_k t}{\hbar} \right) \sigma(X(t)) \quad (\text{A2})$$

(note that $\sigma(X(t))$ is state independent) and $\sigma(X(t))$ satisfies the following integral equation [8]:

$$\sigma(t, t_0) = 1 - \frac{\Gamma^\downarrow}{\hbar} \int_{t_0}^t ds_1 \int_{t_0}^{s_1} ds_2 \sigma(s_1, s_2) \sigma(s_2, t_0) P_\beta(s_1 - s_2) G \left(\frac{X(s_1) - X(s_2)}{X_0} \right). \quad (\text{A3})$$

In the following we shall consider that $t_0 = 0$. Here $P_\beta(s)$ is the fourier transform of the matrix band form-factor in the correlator $\overline{[h_1(X)]_{ij} [h_1(Y)]_{kl}}$, defined in Eq. (2.4):

$$P_\beta(s) = P_\beta^*(-s) = \frac{\kappa_0}{\sqrt{2\pi\hbar}} \exp \left[-\frac{\kappa_0^2}{2\hbar^2} \left(s + i\frac{\hbar\beta}{2} \right)^2 \right], \quad (\text{A4})$$

The influence functional can be determined by solving the following evolution equation:

$$\begin{aligned} \mathcal{L}(X(t_1), Y(t_2)) &= \sigma(t_1, 0) \sigma^*(t_2, 0) + \frac{\Gamma^\downarrow}{\hbar} \int_0^{t_1} ds_1 \int_0^{t_2} ds_2 \mathcal{L}(X(s_1), X(s_2)) \\ &\quad \times P_\beta^*(s_1 - s_2) G \left(\frac{X(s_1) - Y(s_2)}{X_0} \right) \sigma(t_1, s_1) \sigma^*(t_2, s_2). \end{aligned} \quad (\text{A5})$$

APPENDIX B: AVERAGE PROPAGATOR AT FINITE TEMPERATURES

For a given path $X(t)$ the averaged propagator σ satisfies the following equation

$$\sigma(t, t_0) = 1 - \frac{\Gamma^\downarrow}{\hbar} \int_{t_0}^{s_1} ds_1 \int_{t_0}^{s_1} ds_2 \sigma(s_1, s_2) \sigma(s_2, t_0) P_\beta(s_1 - s_2) G \left(\frac{X(s_1) - X(s_2)}{X_0} \right), \quad (\text{B1})$$

where

$$P_\beta(s) = \frac{\kappa_0}{\sqrt{2\pi\hbar}} \exp \left[-\frac{\kappa_0^2}{2\hbar^2} \left(s + i\frac{\hbar\beta}{2} \right)^2 \right] = P_0(s) + \frac{i\beta\hbar}{2} \frac{dP_0(s)}{ds} + \mathcal{O}(\beta^2). \quad (\text{B2})$$

In the above equations $\sigma(s_1, s_2)$ represents the averaged propagator from time s_2 to time s_1 , as for an arbitrary path $X(t)$ it is not obvious that this propagator depends only on the time difference $s_1 - s_2$, as was the case in the adiabatic limit and for $\beta = 0$. We shall assume that the following replacement

$$P_0(s) \equiv \frac{\kappa_0}{\sqrt{2\pi\hbar}} \exp \left[-\frac{\kappa_0^2 s^2}{2\hbar^2} \right] \rightarrow \delta(s) \quad (\text{B3})$$

is legitimate and compute the first correction in β to the propagator.

In the equations for the propagator and the influence functional $P_\beta(s)$ enters under integrals with some arbitrary functions as follows

$$\begin{aligned} \int_{-\infty}^0 ds P_\beta(s) F(s) &\approx \int_{-\infty}^0 ds P_0(s) F(s) + \frac{i\beta\hbar}{2} \int_{-\infty}^0 ds \frac{dP_0(s)}{ds} F(s) \\ &\approx \frac{1}{2} F(0) + \frac{i\beta\kappa_0}{2\sqrt{2\pi}} F(0) - \frac{i\beta\hbar}{4} \left. \frac{dF(s)}{ds} \right|_{s=0}, \end{aligned} \quad (\text{B4})$$

where we have used the following relations

$$\int_{-\infty}^0 ds P_0(s) F(s) = \frac{1}{2} F(0), \quad (\text{B5})$$

$$\int_{-\infty}^0 ds \frac{dP_0(s)}{ds} F(s) = \frac{\kappa_0}{\sqrt{2\pi\hbar}} F(0) - \frac{1}{2} \left. \frac{dF(s)}{ds} \right|_{s=0}, \quad (\text{B6})$$

$$P_0(0) = \frac{\kappa_0}{\sqrt{2\pi\hbar}}. \quad (\text{B7})$$

After a few simple manipulations and after taking into account that

$$\sigma(s, s) = 1, \quad (\text{B8})$$

$$\left. \frac{d\sigma(s_1, s_2)}{ds_1} \right|_{s_1=s_2} = \left. \frac{d\sigma(s_1, s_2)}{ds_2} \right|_{s_1=s_2} = 0, \quad (\text{B9})$$

$$\left. \frac{d}{ds_2} G \left(\frac{X(s_1) - X(s_2)}{X_0} \right) \right|_{s_1=s_2} = \left. \frac{d}{ds_1} G \left(\frac{X(s_1) - X(s_2)}{X_0} \right) \right|_{s_1=s_2} = 0, \quad (\text{B10})$$

one can easily show that up to terms of order $\mathcal{O}(\beta^2)$ the averaged propagator is given by the following expression

$$\sigma(t, 0) = \sigma(t) = \exp \left[-\frac{\Gamma^\downarrow t}{2\hbar} \left(1 + \frac{i\beta\kappa_0}{\sqrt{2\pi}} - \frac{i\beta\Gamma^\downarrow}{4} \right) \right]. \quad (\text{B11})$$

In the equation for the influence functional we shall need the quantity

$$\begin{aligned}\sigma(t)\sigma^*(t') &= \exp \left[-\frac{\Gamma^\downarrow(t+t')}{2\hbar} + \left(\frac{i\beta\kappa_0}{\sqrt{2\pi}} - \frac{i\beta\Gamma^\downarrow}{4} \right) \frac{\Gamma^\downarrow(t-t')}{2\hbar} \right] \\ &\approx \exp \left[-\frac{\Gamma^\downarrow(t+t')}{2\hbar} \right].\end{aligned}\tag{B12}$$

We are allowed to neglect the imaginary contribution in the exponent as in all relevant integrals $t - t' = \mathcal{O}(\beta)$.

APPENDIX C: INFLUENCE FUNCTIONAL AT FINITE TEMPERATURES

In order to simplify somewhat the derivation we shall introduce the “reduced” influence functional at temperature β

$$\Lambda_\beta(X(t_1), Y(t_2)) = \mathcal{L}_\beta(X(t_1), Y(t_2)) \exp \left[\frac{\Gamma^\downarrow(t_1 + t_2)}{2\hbar} \right],\tag{C1}$$

which, up to correction terms of order $\mathcal{O}(\beta^2)$ in the averaged propagators, satisfies the equation

$$\begin{aligned}\Lambda_\beta(X(t_1), Y(t_2)) &= 1 \\ &+ \frac{\Gamma^\downarrow}{\hbar} \int_0^{t_1} ds_1 \int_0^{t_2} ds_2 \Lambda_\beta(X(s_1), Y(s_2)) P_\beta^*(s_1 - s_2) G \left(\frac{X(s_1) - Y(s_2)}{X_0} \right).\end{aligned}\tag{C2}$$

We have shown earlier [8] that for $\beta = 0$

$$\Lambda_0(X(t_1), Y(t_2)) = \Lambda_0(t_1, t_2) = \exp \left\{ \frac{\Gamma^\downarrow}{\hbar} \int_0^{t_<} \left[G \left(\frac{X(s) - Y(s)}{X_0} \right) \right] ds \right\},\tag{C3}$$

where $t_< = \min(t_1, t_2)$. In computing the first order corrections in β for $\Lambda_\beta(X(t_1), Y(t_2))$, we shall proceed as in the previous appendix, by making an expansion

$$P_\beta^*(s) \approx P_0(s) - \frac{i\beta\hbar}{2} \frac{dP_0(s)}{ds}\tag{C4}$$

and taking the limit $\kappa_0 \rightarrow \infty$, which allows us to make the replacement $P_0(s) \rightarrow \delta(s)$ in all the integrals. The only term which requires a more careful treatment in the equation for the reduced influence functional is

$$\beta \frac{\partial \Lambda_\beta(X(s_1), Y(s_2))}{\partial(s_1 - s_2)} \approx \beta \frac{\partial \Lambda_0(X(s_1), Y(s_2))}{\partial(s_1 - s_2)} = \mathcal{O}(\beta^2),\tag{C5}$$

which can thus be neglected. The reason is that $\Lambda_0(X(s_1), Y(s_2))$ has a discontinuous partial derivative at $s_1 - s_2 = 0$. Remembering that we need the influence functional for $t_1 = t_2 = t$ only and by using the obvious exact representation of the integral term

$$\int_0^t ds_1 \int_0^t ds_2 F(s_1, s_2) = \int_0^t ds_1 \int_0^{s_1} ds_2 F(s_1, s_2) + \int_0^t ds_2 \int_0^{s_2} ds_1 F(s_1, s_2)\tag{C6}$$

for an arbitrary function $F(s_1, s_2)$ and by applying the rules described in the previous appendix we obtain that

$$\begin{aligned}\Lambda_\beta(X(t), Y(t)) = & 1 + \frac{\Gamma^\downarrow}{\hbar} \int_0^t ds \Lambda_\beta(X(s), Y(s)) G\left(\frac{X(s) - Y(s)}{X_0}\right) \\ & + \frac{i\beta\Gamma^\downarrow}{4X_0} \int_0^t ds \Lambda_\beta(X(s), Y(s)) [\dot{X}(s) + \dot{Y}(s)] G'\left(\frac{X(s) - Y(s)}{X_0}\right),\end{aligned}\quad (\text{C7})$$

where $G'(x) = dG(x)/dx$. In the above evolution equation one can use either $\Lambda_0(s_1, s_2)$ or $\Lambda_\beta(X(s), Y(s))$ on the r.h.s. An alternative way to derive this equation is to use the fact that for two given paths $X(s_1)$ and $Y(s_2)$ one has the explicit symmetry $\Lambda_0(s_1, s_2) = \Lambda_0(s_2, s_1)$ and also that

$$\frac{dP_0(s)}{ds} = -\frac{dP_0(-s)}{ds} \quad (\text{C8})$$

before making the replacement $P_0(s) \rightarrow \delta(s)$ as described earlier.

This evolution equation can be easily solved as in the case of $\beta = 0$ and the final answer for the influence functional is

$$\begin{aligned}\mathcal{L}(X(t), Y(t)) = & \exp\left\{\frac{\Gamma^\downarrow}{\hbar} \int_0^t ds \left[G\left(\frac{X(s) - Y(s)}{X_0}\right) - 1\right]\right\} \\ & \times \exp\left\{\frac{i\beta\Gamma^\downarrow}{4X_0} \int_0^t ds [\dot{X}(s) + \dot{Y}(s)] G'\left(\frac{X(s) - Y(s)}{X_0}\right)\right\}.\end{aligned}\quad (\text{C9})$$

APPENDIX D: EFFECTIVE HAMILTONIAN AT FINITE TEMPERATURES

Having obtained an expression for the influence functional at finite temperatures we can write down from the Feynman–Vernon path integral an expression for the effective Lagrangian:

$$\begin{aligned}\mathbf{L} = & \frac{M\dot{X}^2}{2} - U(X) - \frac{M\dot{Y}^2}{2} + U(Y) \\ & - i\Gamma^\downarrow \left[G\left(\frac{X - Y}{X_0}\right) - 1\right] + \frac{\beta\Gamma^\downarrow\hbar}{4X_0} [\dot{X} + \dot{Y}] G'\left(\frac{X - Y}{X_0}\right).\end{aligned}\quad (\text{D1})$$

We can introduce now the corresponding canonical conjugate momenta

$$P_X = \frac{\partial \mathbf{L}}{\partial \dot{X}} = M\dot{X} + \frac{\beta\Gamma^\downarrow\hbar}{4X_0} G'\left(\frac{X - Y}{X_0}\right), \quad (\text{D2})$$

$$P_Y = \frac{\partial \mathbf{L}}{\partial \dot{Y}} = -M\dot{Y} + \frac{\beta\Gamma^\downarrow\hbar}{4X_0} G'\left(\frac{X - Y}{X_0}\right) \quad (\text{D3})$$

and construct the effective Hamiltonian according to usual rules

$$\begin{aligned}
\mathbf{H} &= P_X \dot{X} + P_Y \dot{Y} - \mathbf{L} \\
&= \frac{1}{2M} \left[P_X - \frac{\beta \Gamma^\downarrow \hbar}{4X_0} G' \left(\frac{X-Y}{X_0} \right) \right]^2 + U(X) - \frac{1}{2M} \left[P_Y - \frac{\beta \Gamma^\downarrow \hbar}{4X_0} G' \left(\frac{X-Y}{X_0} \right) \right]^2 - U(Y) \\
&\quad + i\Gamma^\downarrow \left[G \left(\frac{X-Y}{X_0} \right) - 1 \right].
\end{aligned} \tag{D4}$$

The requantization of this effective Hamiltonian is straightforward ($P_X \rightarrow -i\hbar\partial_X$ and $P_Y \rightarrow -i\hbar\partial_Y$) and it is convenient to reorder the different terms in the Hamiltonian as follows:

$$\begin{aligned}
\mathbf{H} &= \frac{(P_X + P_Y)(P_X - P_Y)}{2M} + U(X) - U(Y) \\
&\quad - \frac{\beta \Gamma^\downarrow \hbar}{4MX_0} G' \left(\frac{X-Y}{X_0} \right) (P_X - P_Y) + i\Gamma^\downarrow \left[G \left(\frac{X-Y}{X_0} \right) - 1 \right].
\end{aligned} \tag{D5}$$

Any other choice of ordering leads to an evolution equation for the density matrix $\rho(X, Y, t)$ which does not conserve probability. One can consider alternative orderings, but in the final analysis these lead to slight renormalizations of various quantities, but to no qualitative effects.

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Table I. The definition of our parameters as well as some of the limits used in this analysis.

Parameters:

X_0 Characteristic scale over which $H_1(X)$ changes.

N Dimension of the Hilbert space of the intrinsic subsystem. We take the limit $N \gg 1$.

κ_0 The bandwidth of the random matrix $H_1(X)$. The average number of states coupled together at a given excitation energy is determined by the density of states: $N_0 \sim \kappa_0 \rho(\varepsilon)$. For $\kappa_0 \rightarrow \infty$, we recover the full random matrix limit.

Γ^\downarrow Spreading width. For an initially uncorrelated state evolving under a random matrix, the average propagator decays as $\sigma(t) \sim \exp(-\Gamma^\downarrow t/2\hbar)$.

$\beta = 1/T$ Inverse thermodynamic temperature, defined through the density of states.

$\rho(\varepsilon)$ The density of states. We use the form $\rho(\varepsilon) = \rho_0 \exp(\beta\varepsilon)$. When $\beta = 0$, the intrinsic system has a constant level density.

$G(x)$ Correlation function for the intrinsic states. It describes how far one must go in X before the intrinsic states are statistically uncorrelated. Typically one can use $G(x) = \exp(-x^2/2)$, $1 - x^2/2$ or $\cos x$.

γ Friction coefficient obtained in the classical limit and in the full quantum dynamical solution, given by $\gamma = \beta\Gamma^\downarrow\hbar/2MX_0^2$.

D Diffusion constant, given by $D = 2X_0^2/\beta^2\Gamma^\downarrow\hbar$.

Limits:

$X_0 \rightarrow \infty$ Weak coupling limit.

$\left. \begin{array}{l} \hbar/X_0 \rightarrow 0 \\ X_0/\Gamma^\downarrow \rightarrow 0 \\ \gamma = \text{finite} \end{array} \right\}$ Brownian motion limit.

$\hbar \rightarrow 0$ Classical Limit.

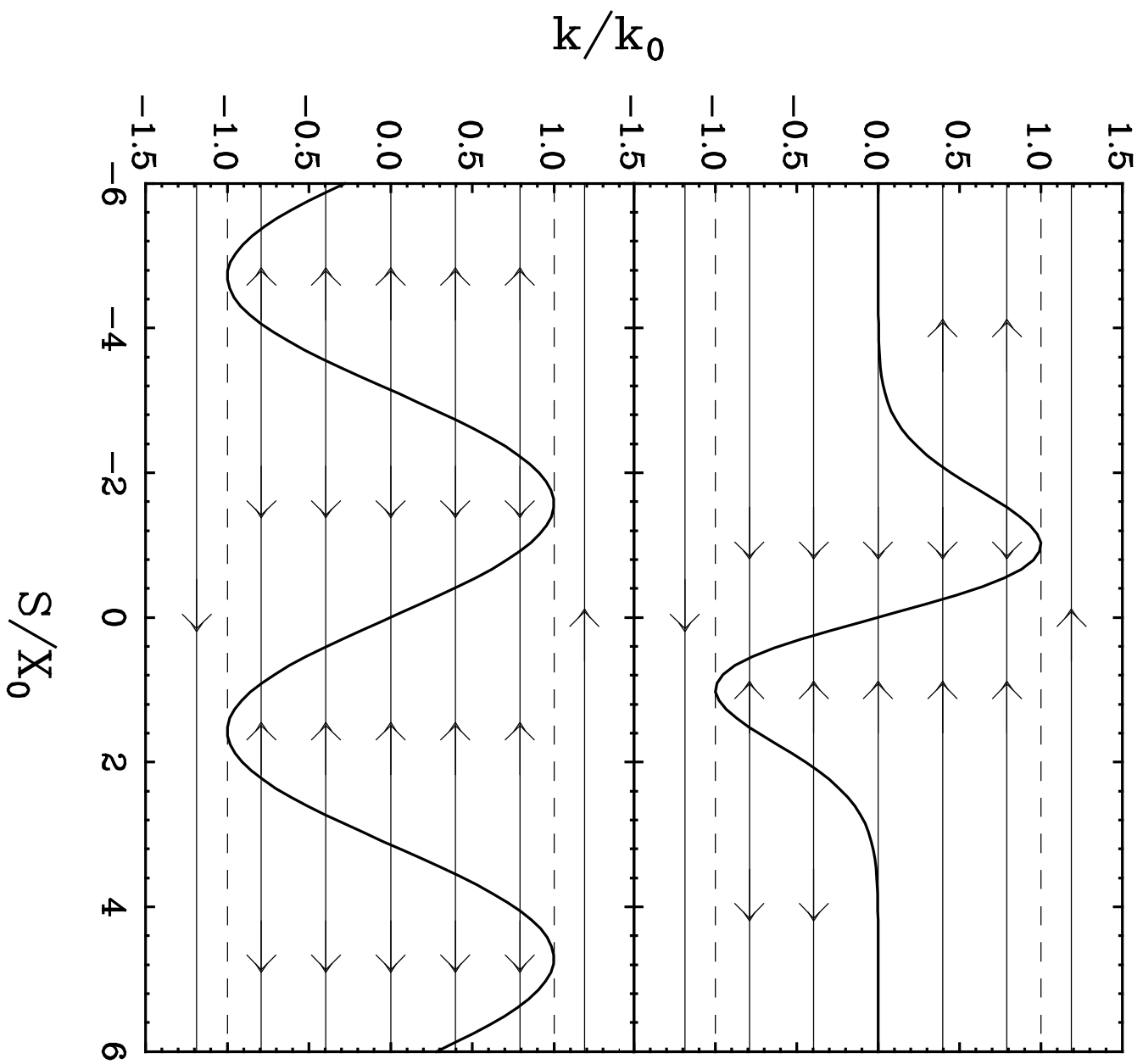
$\kappa_0 \rightarrow \infty$ Adiabatic Limit. This implies that the collective time scale X_0/V is much longer than the intrinsic one given by \hbar/κ_0 .

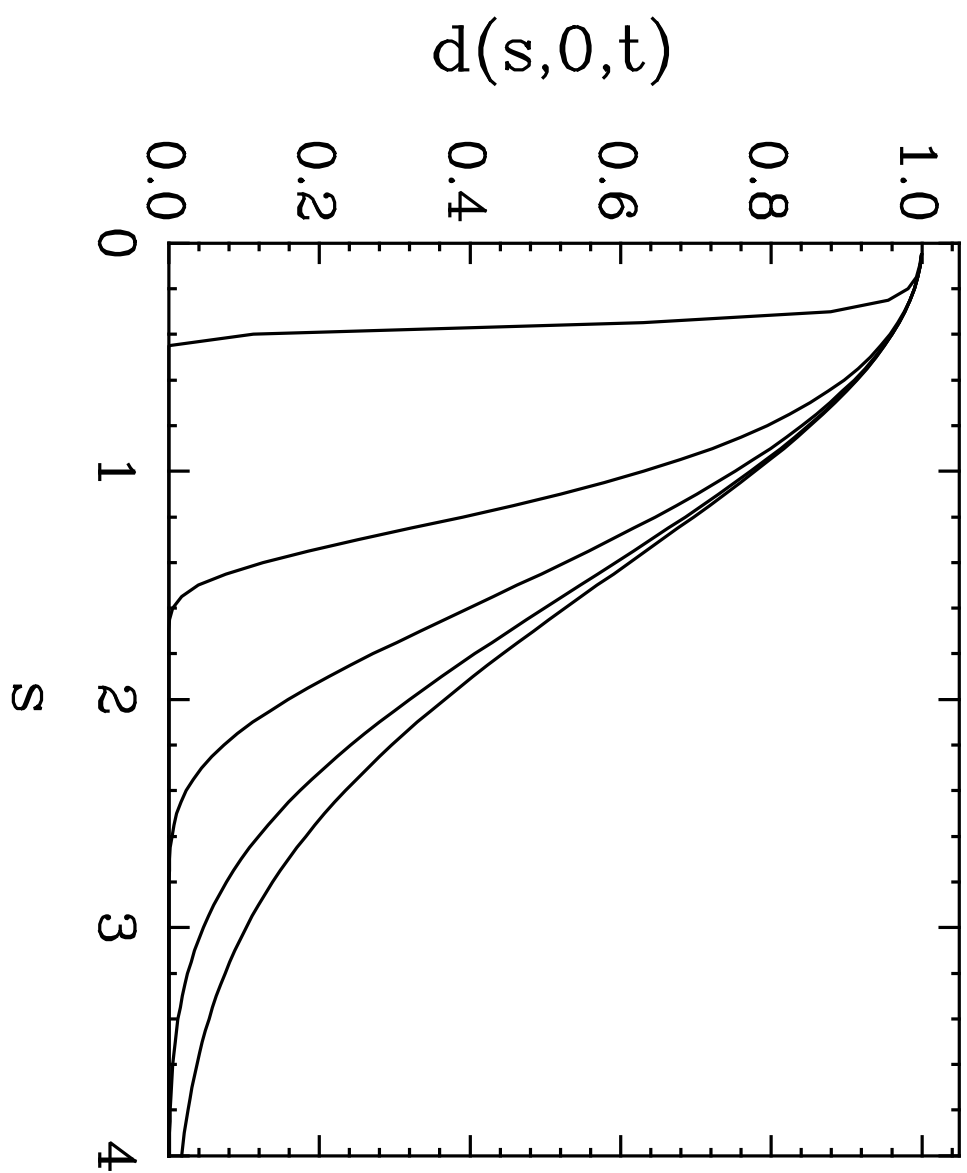
Figure Captions

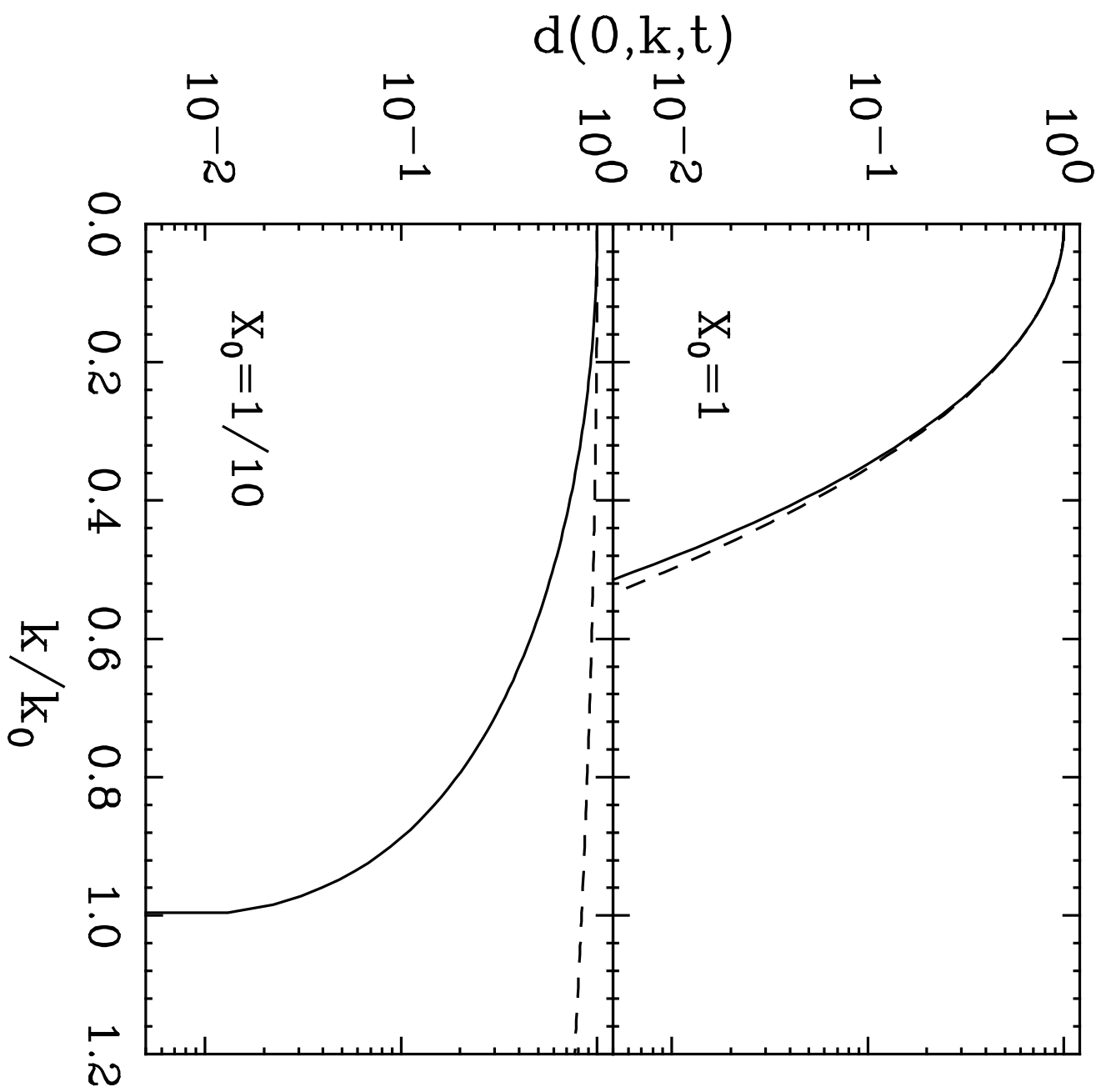
- Figure 1. Time dependent flow $S(t)$ associated with the time evolution of the density matrix in a linear potential. (top) The case of a Gaussian correlation $G(x) = \exp[-x^2/2]$. (bottom) The flow for a periodic correlation function $G(x) = \cos[x]$. The stability of the lines of fixed points are indicated by the directions of the arrows.
- Figure 2. Fourier transform of the momentum distribution, $d(s, 0, t)$, as a function of s , for $F = 0$ and $M = \hbar = \beta = 1$. From narrowest to widest we have $X_0 = 0.1, 0.5, 1, 2, \infty$. The $X_0 = \infty$ (widest curve) is a Gaussian distribution.
- Figure 3. Fourier transform of the coordinate distribution $d(0, k, t)$ for the case of a linear potential. The solid curve is the result obtained from Eqs. 5.5 and 5.7 from integration to $t = 100$. This is compared to a Gaussian (dashes) obtained from the second cumulant alone. The top and bottom correspond to different correlation lengths $X_0 = 1$ and $X_0 = 1/10$.
- Figure 4. Time dependent flow $(S(t), K(t))$ associated with the time evolution of the density matrix in a harmonic oscillator potential, with the correlation function $G(x) = \exp[-x^2/2]$. The values of the parameters are $\omega = 1$ and $\gamma = 0.1$ (top) and $\gamma = 0.5$ (bottom).
- Figure 5. Eigenvalue spectrum for the time-evolution operator of the density matrix $\rho(r, s, t)$ for the harmonic oscillator with $\beta > 0$. For $\beta = 0$, the friction γ vanishes, and all eigenvalues lie on the real axis. The $\lambda = 0$ solution corresponds to the equilibrium density matrix.
- Figure 6. Fourier transform of the momentum and coordinate distribution (they coincide in this case) for the harmonic oscillator for the case $M = \hbar = \omega = \beta = 1$ here represented as a function of \sqrt{I} , where I is the action. The curves correspond to $X_0 = 0.5, 1, 2, \infty$ from the narrowest to the widest. The Gaussian distribution ($X_0 = \infty$), obtained from the Brownian motion limit in which only the quadratic cumulant is non-zero, is shown as a dashed curve.
- Figure 7. Time dependent flow associated with the time evolution of the density matrix in an inverted harmonic oscillator potential, with the correlation function $G(x) = \exp(-x^2/2)$. The parameters are $\omega = 1/10$ and $\gamma = 1/2$. The flow of certain trajectories are shown with the arrows.
- Figure 8. Double well potential and eigenstates in the absence of the coupling to the intrinsic degrees of freedom.
- Figure 9. Strengths tunneled to the right hand well for $\Gamma^\downarrow = 0.5, 1$ and π (upward from the lowest curve) and $\beta = 0$.
- Figure 10. Strengths tunneled to the right hand well for $\Gamma^\downarrow = \pi$ and $\beta = 0, 0.05, 0.10, 0.15, 0.20$ (downward from the highest curve).

Figure 11. Density distributions at $t=0$ (the narrowest curve) and at time $t=4$ for $X_0 = 0.2$, $\beta = 0$, $\Gamma^\downarrow = 1$: the continuous (dotted) curve corresponds to using the quadratic (Gaussian) correlation function.

Figure 12. (Top) Temperature behavior of the complex eigenvalues of the double well potential with the smallest imaginary parts. (Bottom) Temperature dependence of the imaginary part of the eigenvalues with smallest absolute value. One of the eigenvalues apparently vanishes in the limit $T \rightarrow 0$, which suggests that at $T = 0$ dissipation decreases the tunnelling rate [2]. One can see that the tunneling process is not always dominated by a single eigenvalue.







K

